



# Full wwPDB X-ray Structure Validation Report

Nov 23, 2014 – 12:52 PM EST

PDB ID : 4W2B  
Title : Crystal structure of the peptolide 12C bound to bacterial ribosome  
Authors : Fagan, C.E.; Dunham, C.M.  
Deposited on : 2014-03-24  
Resolution : 3.60 Å(reported)

This is a full wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

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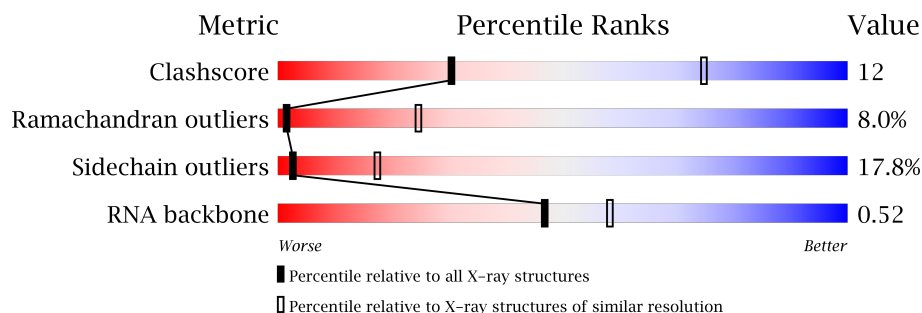
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable24195

# 1 Overall quality at a glance

The reported resolution of this entry is 3.60 Å.

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



| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| Clashscore            | 79885                       | 1155 (3.80-3.40)                                      |
| Ramachandran outliers | 78287                       | 1109 (3.80-3.40)                                      |
| Sidechain outliers    | 78261                       | 1108 (3.80-3.40)                                      |
| RNA backbone          | 1838                        | 1012 (4.40-2.76)                                      |







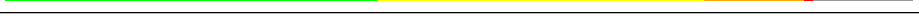

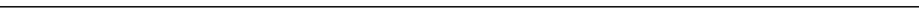
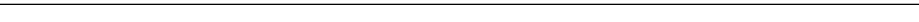








The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 2915   |                  |
| 2   | B     | 122    |                  |
| 3   | C     | 276    |                  |
| 4   | D     | 206    |                  |
| 5   | E     | 210    |                  |
| 6   | F     | 182    |                  |
| 7   | G     | 180    |                  |
| 8   | H     | 148    |                  |
| 9   | I     | 140    |                  |
| 10  | J     | 122    |                  |
| 11  | K     | 150    |                  |
| 12  | L     | 141    |                  |
| 13  | M     | 118    |                  |
| 14  | N     | 112    |                  |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 15  | O     | 146    |  |
| 16  | P     | 118    |  |
| 17  | Q     | 101    |  |
| 18  | R     | 113    |  |
| 19  | S     | 96     |  |
| 20  | T     | 110    |  |
| 21  | U     | 206    |  |
| 22  | V     | 85     |  |
| 23  | W     | 98     |  |
| 24  | X     | 72     |  |
| 25  | Y     | 60     |  |
| 26  | Z     | 71     |  |
| 27  | a     | 60     |  |
| 28  | b     | 54     |  |
| 29  | c     | 49     |  |
| 30  | d     | 65     |  |
| 31  | e     | 37     |  |
| 32  | f     | 12     |  |

## 2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 92290 atoms, of which 0 are hydrogen and 0 are deuterium.

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

- Molecule 1 is a RNA chain called 23S ribosomal RNA.

| Mol | Chain | Residues | Atoms |       |       |       |      | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
| 1   | A     | 2882     | Total | C     | N     | O     | P    | 0       | 0       | 0     |
|     |       |          | 62071 | 27627 | 11611 | 19952 | 2881 |         |         |       |

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

| Mol | Chain | Residues | Atoms |      |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|---------|-------|
| 2   | B     | 120      | Total | C    | N   | O   | P   | 0       | 0       | 0     |
|     |       |          | 2573  | 1146 | 476 | 832 | 119 |         |         |       |

- Molecule 3 is a protein called 50S ribosomal protein L2.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 3   | C     | 272      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2115  | 1335 | 420 | 357 | 3 |         |         |       |

- Molecule 4 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 4   | D     | 205      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1568  | 991 | 300 | 271 | 6 |         |         |       |

- Molecule 5 is a protein called 50S ribosomal protein L4.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 5   | E     | 202      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1585  | 1011 | 297 | 275 | 2 |         |         |       |

- Molecule 6 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 6   | F     | 181      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1474  | 942 | 268 | 260 | 4 |         |         |       |

- Molecule 7 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 7   | G     | 170      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1307  | 829 | 245 | 232 | 1 |         |         |       |

- Molecule 8 is a protein called 50S ribosomal protein L9.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8   | H     | 146      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1136  | 726 | 201 | 208 | 1 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 9   | I     | 138      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1104  | 712 | 206 | 182 | 4 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10  | J     | 122      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 933   | 588 | 171 | 170 | 4 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 11  | K     | 150      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1145  | 712 | 232 | 198 | 3 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 12  | L     | 141      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1122  | 715 | 212 | 188 | 7 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 13  | M     | 118      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 968   | 604 | 203 | 160 | 1 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 14  | N     | 111      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 882   | 556 | 176 | 150 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 15  | O     | 137      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1141  | 710 | 234 | 196 | 1 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 16  | P     | 117      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 964   | 610 | 202 | 151 | 1 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 17  | Q     | 101      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 779   | 501 | 142 | 135 | 1 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 18  | R     | 113      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 900   | 566 | 177 | 155 | 2 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 19  | S     | 92       | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 725   | 471 | 131 | 123 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 20  | T     | 102      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 785   | 505 | 150 | 125 | 5 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 21  | U     | 183      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1461  | 933 | 260 | 265 | 3 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 22  | V     | 82       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 648   | 401 | 138 | 108 | 1 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 23  | W     | 97       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 763   | 481 | 150 | 131 | 1 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 24  | X     | 69       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 581   | 358 | 118 | 104 | 1 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 25  | Y     | 59       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 469   | 298 | 90 | 81 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 26  | Z     | 71       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 581   | 364 | 108 | 104 | 5 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 27  | a     | 59       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 459   | 288 | 90 | 76 | 5 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 28  | b     | 49       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 424   | 264 | 87 | 69 | 4 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 29  | c     | 49       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 430   | 263 | 108 | 57 | 2 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 30  | d     | 64       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 517   | 331 | 102 | 82 | 2 |         |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 31  | e     | 37       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 307   | 188 | 68 | 47 | 4 |         |         |       |

- Molecule 32 is a protein called T17-GLY-GLY-PRO-LYS-LYS-LYS-LYS-LYS-VAL-GLY-GLY.

| Mol | Chain | Residues | Atoms |    |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|---------|-------|
| 32  | f     | 9        | Total | C  | N  | O  | 0       | 0       | 0     |
|     |       |          | 116   | 78 | 18 | 20 |         |         |       |

- Molecule 33 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 33  | P     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 33  | D     | 2        | Total | Mg | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 33  | K     | 3        | Total | Mg | 0       | 0       |
|     |       |          | 3     | 3  |         |         |
| 33  | E     | 1        | Total | Mg | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 33  | B     | 2        | Total | Mg | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 33  | C     | 3        | Total | Mg | 0       | 0       |
|     |       |          | 3     | 3  |         |         |

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| Mol | Chain | Residues | Atoms        |           | ZeroOcc | AltConf |
|-----|-------|----------|--------------|-----------|---------|---------|
| 33  | V     | 1        | Total<br>1   | Mg<br>1   | 0       | 0       |
| 33  | A     | 243      | Total<br>243 | Mg<br>243 | 0       | 0       |

- Molecule 34 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms      |         | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 34  | a     | 1        | Total<br>1 | Zn<br>1 | 0       | 0       |

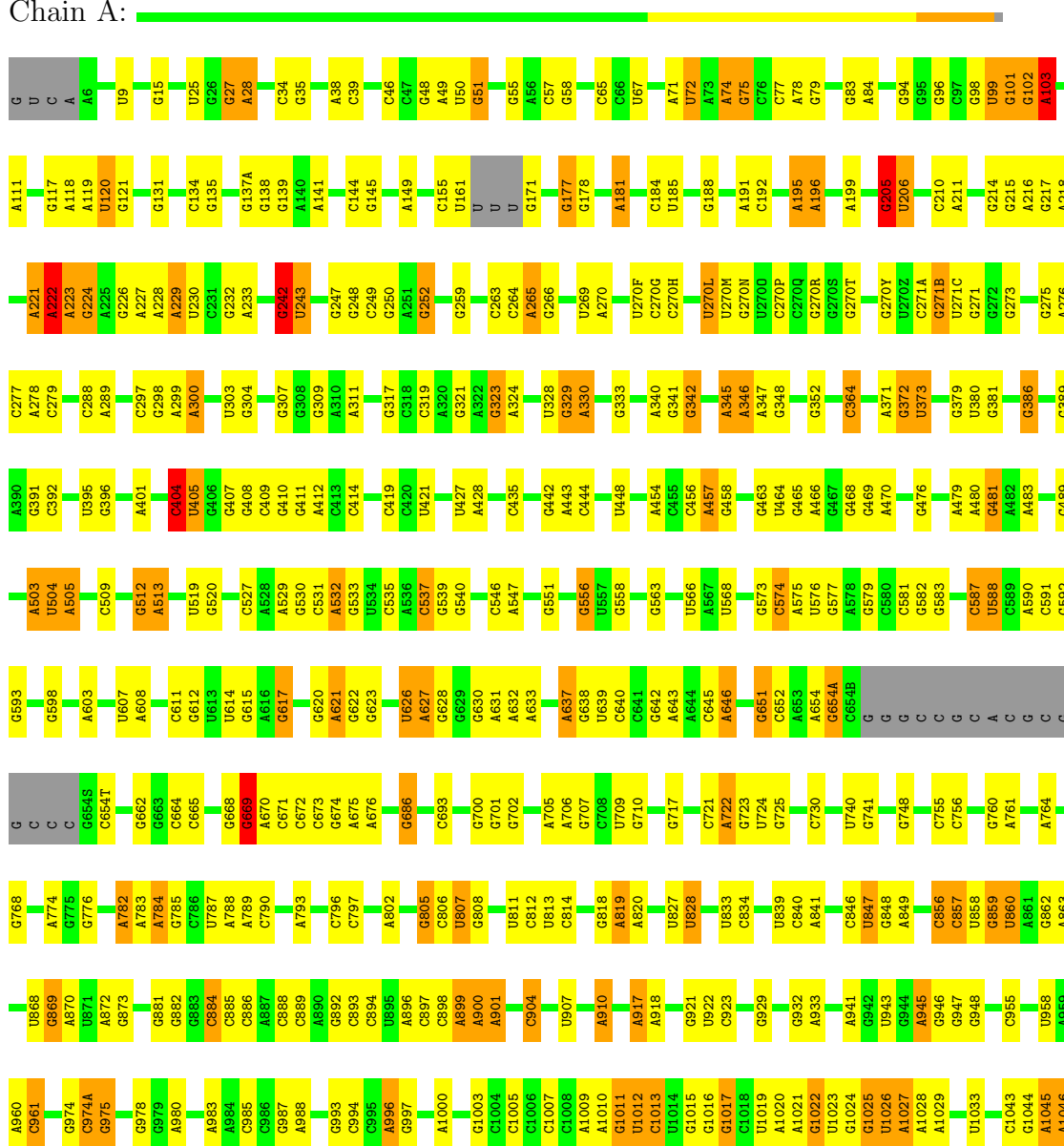
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron 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 dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

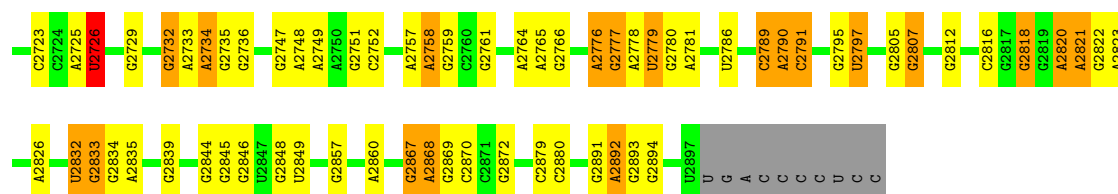
Note EDS was not executed.

#### • Molecule 1: 23S ribosomal RNA

Chain A:

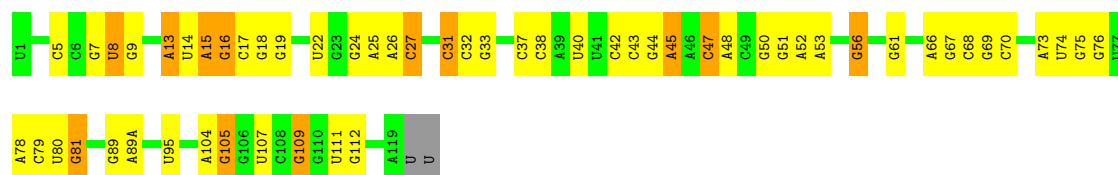


|       |       |       |       |       |       |       |       |       |       |       |        |       |        |       |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|--------|-------|--------|-------|
| G2627 | A2518 | G2405 | C2313 | A2212 | G2121 | U2011 | G1899 | U1777 | C1638 | G1519 | U1420  | U1316 | C1221  | G1047 |
| G2628 | U2519 | U2406 | C2314 | U2213 | U2122 | G2012 | G1899 | A1780 | U1639 | G1522 | G1421  | A1317 | G1226  | A1048 |
| A2629 | C2520 |       | G2315 | G2215 | G2123 | A2019 | C1902 | C1782 | C1640 | G1527 | A1427  | A1321 | G1227  | C1049 |
| G2630 |       |       | G2316 | G2216 | G2124 |       | C1906 |       | C1642 |       | G1428  | A1322 | G1228  | A1050 |
| A2631 | C2527 |       | C2317 | G2224 | A2125 | U2022 | A1913 | A1787 | C1646 | C1533 | G1429  | U1329 | G1231  | C1052 |
| G2632 | U2528 |       | G2318 | A2225 | G2126 | G2023 | A1919 |       | C1647 | C1534 | C1430  | G1330 | G1232  | C1053 |
| G2633 | G2529 |       | G2319 | C2226 | G2127 |       | C1920 | C1790 | C1648 | U1535 | U1431  | A1331 | G1138  | A1054 |
| G2634 |       |       | A2320 | A2227 | C2128 | G2030 | A1918 | A1791 | C1649 | U1536 | G1441  | G1332 | G1139  | G1055 |
| U2537 | U2538 |       | G2321 |       |       | A2030 | C1920 | C1795 | G1653 | C1537 | G1442  | U1336 | U1140  | G1056 |
| A2542 |       |       | A2322 | G2238 | G2131 | A2031 | C1921 | U1796 | A1654 | G1538 | G1443  | G1337 | U1142  | G1057 |
| G2543 | G2543 |       | G2323 | G2239 | U2132 | G2032 | C1922 | C1797 | A1664 | G1542 | A1444A | G1338 | A1142A | G1058 |
| G2544 |       |       | G2324 |       | G2133 | A2033 | G1929 | U1798 | G1667 | A1543 | C1445  | U1341 | G1244  | U1060 |
| U2547 |       |       | C2325 | G2240 | G2134 | G2038 | C1930 | G1799 |       | A1544 |        |       | G1245  | U1061 |
| U2548 | U2548 |       | C2326 | U2243 | U2144 | C2043 | U1931 | A1801 | G1674 | A1545 | G1449  | G1348 | G1252  | G1062 |
| U2555 |       |       | G2330 | U2244 | C2145 | C2050 | U1936 | G1802 | C1675 | C1547 | A1453  | A1349 | G1253  | C1064 |
| G2556 |       |       | G2331 | U2245 | C2146 | A2051 | A1937 | A1803 | C1676 | C1548 | U1454  | A1353 | U1255  | U1065 |
|       |       |       |       | A2247 | G2147 | G2052 | A1938 | G1804 | A1678 |       | G1455  | U1357 | G1256  | U1066 |
|       |       |       |       |       | G2148 | A2054 | U1939 | U1805 | G1677 | A1558 |        | U1357 | G1259  | G1068 |
| U2562 | U2563 |       | A2336 | U2262 | U2150 | C2055 | C1942 | A1809 | U1688 | A1569 | G1458  | G1358 | G1260  | A1069 |
| U2564 |       |       | U2344 | C2263 | G2151 | G2056 | U1943 |       | U1689 |       | C1459  | A1359 | G1264  | G1071 |
| A2565 |       |       | G2345 |       |       | A2057 | U1943 |       | A1689 |       | A1460  |       | G1264  | C1076 |
| U2566 |       |       | A2346 | A2268 | G2154 | A2058 | A1952 | A1812 | A1690 | C1577 | G1461  | C1363 | A1265  | C1077 |
| G2567 |       |       | C2347 | A2269 | G2155 | G2059 | A1952 | G1813 |       | U1578 |        | G1364 | G1170  | U1077 |
|       |       |       |       |       | G2156 | A2060 | U1955 |       | U1693 | A1579 | C1467  | A1365 | U1267  | U1078 |
| G2569 |       |       | C2350 | G2271 | G2157 | G2061 | U1955 | G1816 | C1694 | A1580 | C1468  | A1366 | U1267  | C1079 |
|       |       |       |       |       | A2158 | A2062 | C1962 | A1819 | G1695 |       | G1469  | A1367 | U1269  | G1080 |
| G2575 |       |       | G2354 | C2275 |       |       | C1962 | U1820 |       | C1585 | G1470  | G1368 | G1270  | U1081 |
| G2576 |       |       |       | G2276 | G2162 | U2068 | U1963 |       | U1696 | A1586 | A1471  | G1369 | G1271  | U1082 |
|       |       |       | C2364 | G2277 | C2163 | G2069 | G1964 | C1827 | G1725 |       | G1479  | G1370 | G1272  | U1083 |
| C2579 |       |       |       |       | G2165 | A2071 | C1967 | A1828 |       | G1591 | G1480  | U1372 | U1273  | U1084 |
| G2581 |       |       | A2369 | G2282 | G2166 |       | G1968 | A1829 | G1728 | C1592 | U1482  | A1373 | U1273  | A1085 |
| G2582 |       |       |       | C2283 | U2167 | U2086 | A1969 |       | A1729 | G1593 | G1483  |       | A1278  | A1086 |
|       |       |       | A2376 | C2284 | G2168 | G2087 | A1970 | G1835 | U1730 | G1594 | G1484  | A1379 | A1287  | G1087 |
|       |       |       | A2377 | C2285 | G2169 |       | A1971 |       | G1731 | G1595 | G1485  | A1380 | U1288  | A1088 |
| C2586 |       |       | G2379 | A2287 | A2170 | G2093 | A1972 | A1847 | G1732 |       |        |       |        |       |
|       |       |       |       |       | A2171 |       |       | A1848 | A1733 | C1598 |        |       |        |       |
| C2601 |       |       | G2383 | U2291 | U2172 | U2099 | G1980 |       | G1742 |       | A1490  | A1384 | C1291  | G1091 |
| A2602 |       |       |       | C2292 | A2173 | G2100 | A1981 | G1858 | G1743 | A1603 | G1491  | G1385 | U1292  | C1092 |
| G2603 |       |       | C2385 | C2293 |       | G2101 | C1982 | A1859 |       |       | G1492  | C1386 | C1293  | G1093 |
| U2604 |       |       | G2386 | C2294 | A2176 | U2102 | G1989 | G1861 | C1752 | C1607 | A1494  |       |        | U1094 |
| C2606 |       |       | U2387 | C2295 | A2177 | C2103 | G1989 |       | G1753 | A1608 | A1495  | U1394 | G1297  | A1095 |
|       |       |       | A2388 |       | G2186 |       | G1990 | U1864 | G1754 | A1609 | U1497  | C1403 | C1299  | A1096 |
| U2609 |       |       | G2389 | G2298 | G2187 | C2107 | G1991 | G1869 | A1755 | A1610 | C1498  |       | G1195  |       |
| C2610 |       |       | U2390 |       | C2188 |       | G1992 | C1870 | G1756 | A1614 |        | C1407 | U1300  | U1101 |
| U2611 |       |       | G2391 |       | U2189 | C2111 | U1993 | A1871 |       | C1615 | C1505  | C1408 | A1301  | A1103 |
| G2612 |       |       | A2392 | G2303 | G2190 | G2112 | C1994 | A1872 | G1758 | G1616 |        |       | A1204  | G1110 |
| U2613 |       |       | C2393 | G2304 | G2191 | U2113 | U1995 | A1878 |       | A1506 | A1507  | A1412 | G1308  | G1111 |
| A2614 |       |       | G2394 | A2305 | G2192 | A2114 | C1996 | G1878 | G1763 | A1617 | A1508  | G1413 | A1309  | G1112 |
|       |       |       | C2395 | C2306 | G2115 | G2116 | G2006 |       | G1764 | A1618 | C1509  |       | G1310  |       |
| C2617 |       |       | G2396 | G2307 | A2198 | G2117 | C2007 | C1881 |       | G1622 | U1510  | G1416 | G1209  | G1122 |
|       |       |       |       | G2308 | A2199 | U2118 | C2008 | C1882 |       |       |        | C1417 | A1210  |       |
|       |       |       | C2402 |       | G2210 | A2119 | C2008 |       | A1773 | C1636 | U1514  | G1418 | U1211  | G1125 |
| G2623 |       |       | C2403 | A2311 | G2210 | A2119 | G2009 | G1888 | C1774 | A1637 |        |       |        | G1126 |
| C2626 |       |       | C2404 | U2312 | G2211 | G2120 | G2010 | A1889 |       |       |        |       | A1419  | A1126 |



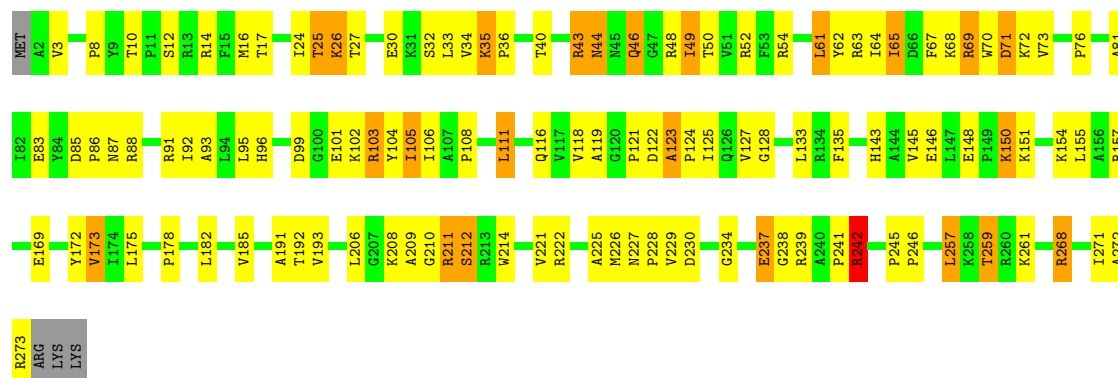
• Molecule 2: 5S ribosomal RNA

Chain B:



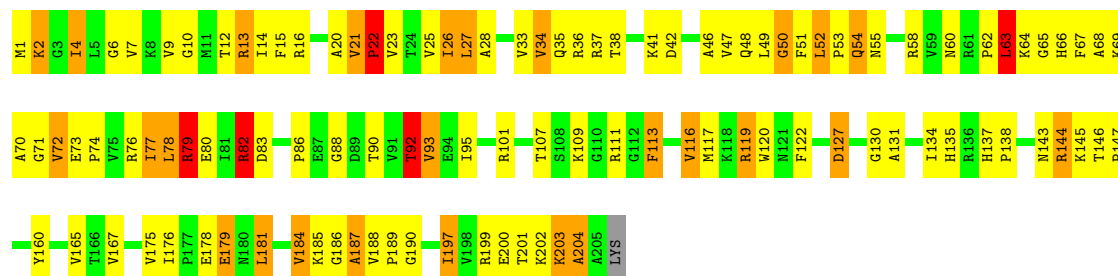
• Molecule 3: 50S ribosomal protein L2

Chain C:



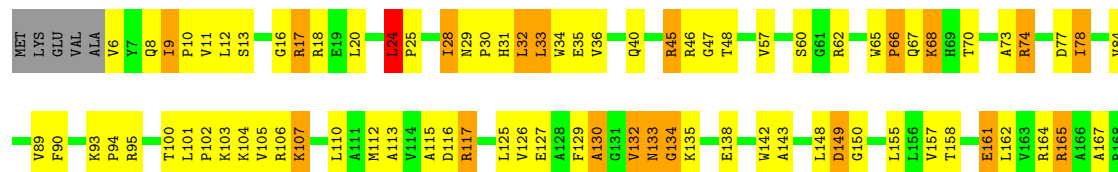
• Molecule 4: 50S ribosomal protein L3

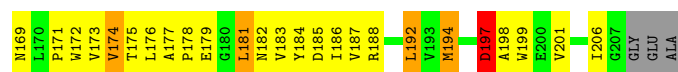
Chain D:



• Molecule 5: 50S ribosomal protein L4

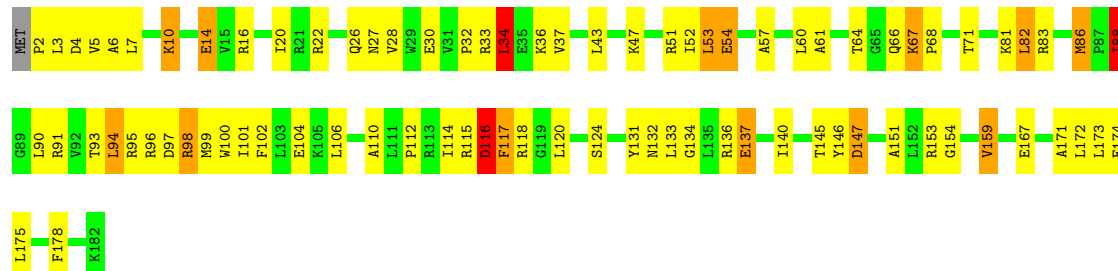
Chain E:





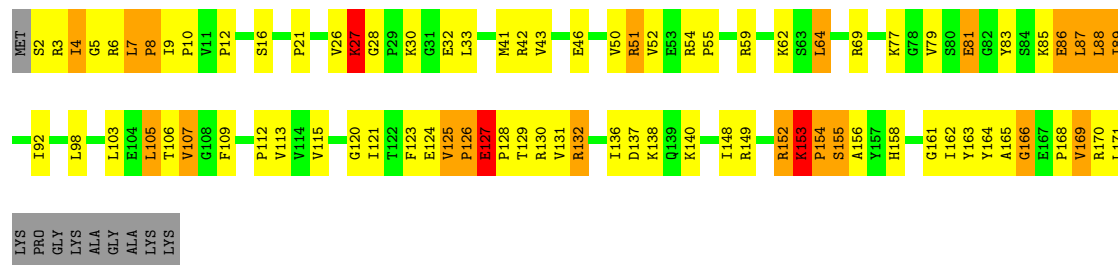
• Molecule 6: 50S ribosomal protein L5

Chain F:



• Molecule 7: 50S ribosomal protein L6

Chain G:



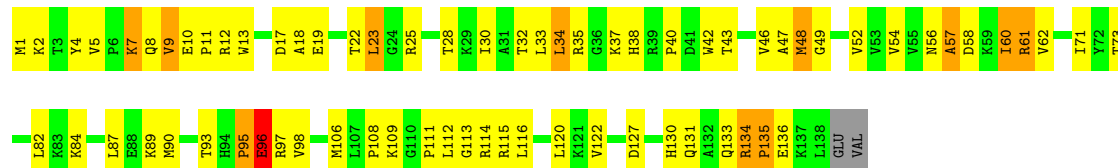
• Molecule 8: 50S ribosomal protein L9

Chain H:



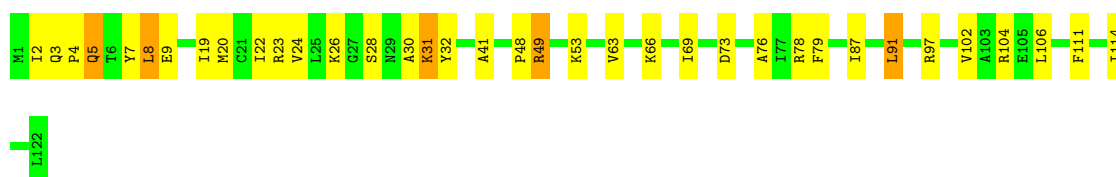
• Molecule 9: 50S ribosomal protein L13

Chain I:



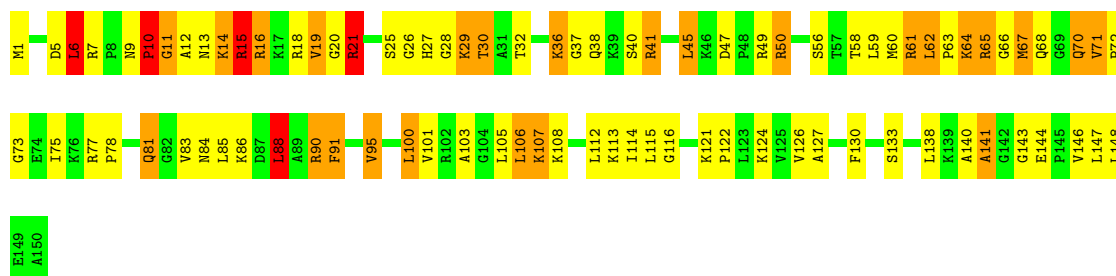
• Molecule 10: 50S ribosomal protein L14

Chain J:



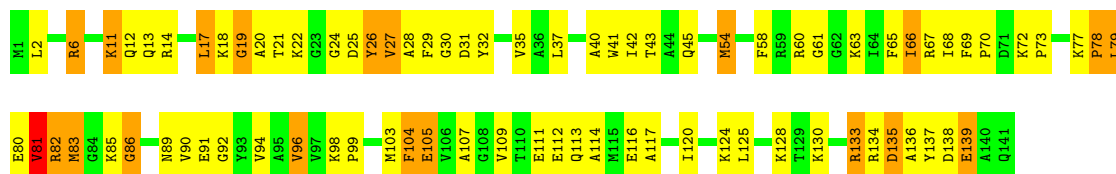
- Molecule 11: 50S ribosomal protein L15

Chain K:



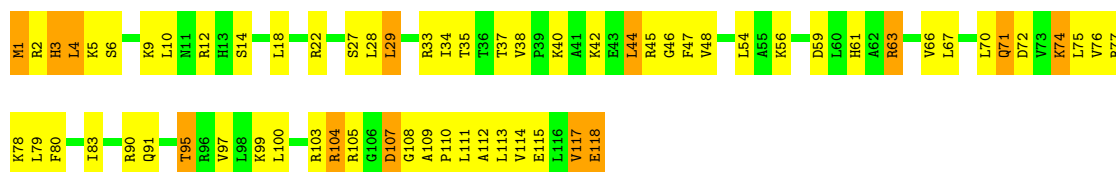
- Molecule 12: 50S ribosomal protein L16

Chain L:



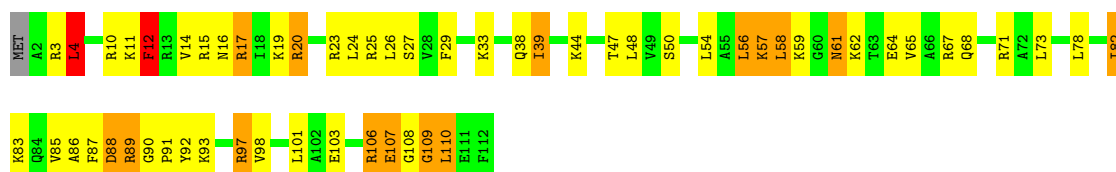
- Molecule 13: 50S ribosomal protein L17

Chain M:



- Molecule 14: 50S ribosomal protein L18

Chain N:



- Molecule 15: 50S ribosomal protein L19

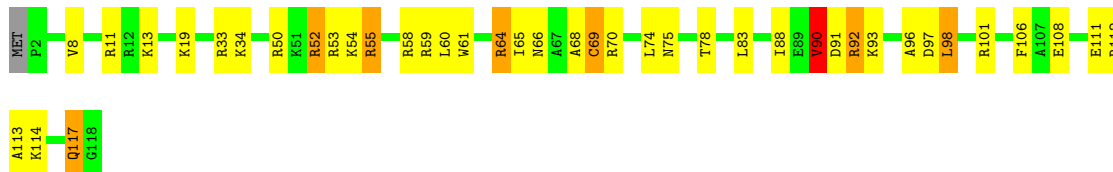
Chain O:





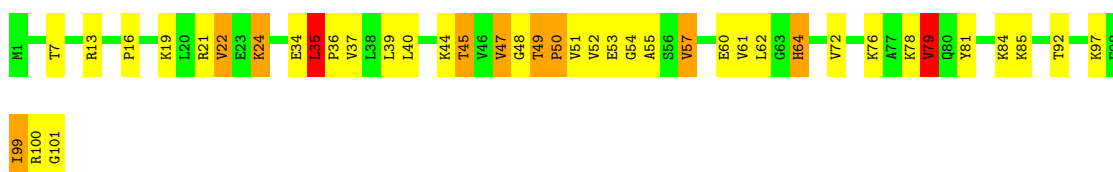
- Molecule 16: 50S ribosomal protein L20

Chain P:



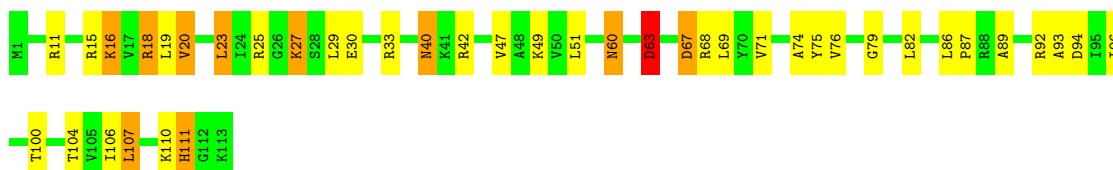
- Molecule 17: 50S ribosomal protein L21

Chain Q:



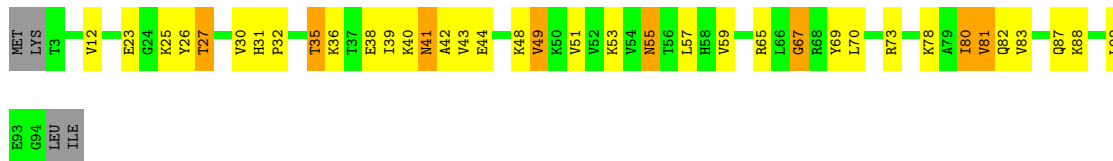
- Molecule 18: 50S ribosomal protein L22

Chain R:



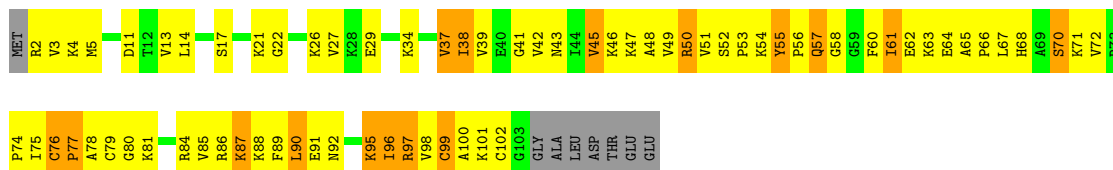
- Molecule 19: 50S ribosomal protein L23

Chain S:



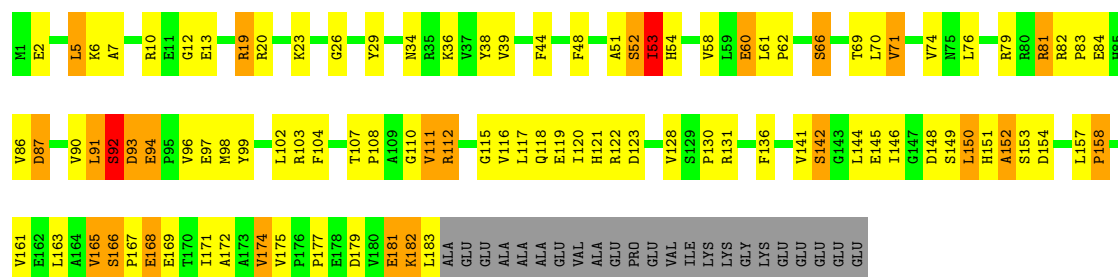
- Molecule 20: 50S ribosomal protein L24

Chain T:



- Molecule 21: 50S ribosomal protein L25

Chain U: 



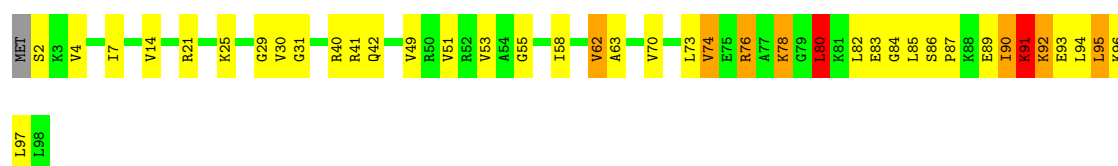
- Molecule 22: 50S ribosomal protein L27

Chain V: 



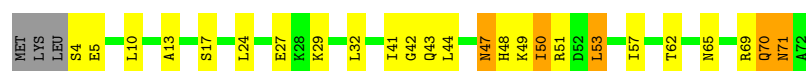
- Molecule 23: 50S ribosomal protein L28

Chain W: 



- Molecule 24: 50S ribosomal protein L29

Chain X: 



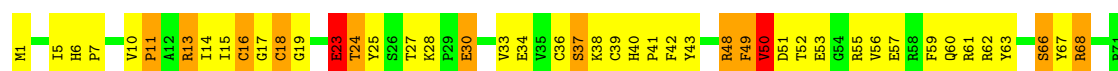
- Molecule 25: 50S ribosomal protein L30

Chain Y: 



- Molecule 26: 50S ribosomal protein L31

Chain Z: 



- Molecule 27: 50S ribosomal protein L32

Chain a: 



- Molecule 28: 50S ribosomal protein L33



Chain b: 



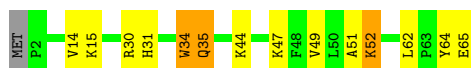
- Molecule 29: 50S ribosomal protein L34

Chain c: 



- Molecule 30: 50S ribosomal protein L35

Chain d: 



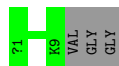
- Molecule 31: 50S ribosomal protein L36

Chain e: 



- Molecule 32: T17-GLY-GLY-PRO-LYS-LYS-LYS-LYS-LYS-VAL-GLY-GLY

Chain f: 



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

| Property   | Value   | Source    |
|--|---|-----------|
| Space group  | P 21 21 21                                      | Depositor |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$ | 209.24Å 443.46Å 618.62Å<br>90.00° 90.00° 90.00° | Depositor |
| Resolution (Å)   | 49.79 – 3.60                                    | Depositor |
| % Data completeness<br>(in resolution range)             | 98.1 (49.79-3.60)                               | Depositor |
| $R_{merge}$  | (Not available)                                 | Depositor |
| $R_{sym}$  | (Not available)                                 | Depositor |
| Refinement program                                       | PHENIX (phenix.refine: 1.8.3_1479)              | Depositor |
| R, $R_{free}$  | 0.222 , 0.254                                   | Depositor |
| Estimated twinning fraction                              | No twinning to report.                          | Xtriage   |
| Total number of atoms                                    | 92290   | wwPDB-VP  |
| Average B, all atoms (Å <sup>2</sup> )                   | 114.0   | wwPDB-VP  |

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, T17, MG

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   | A     | 0.26         | 0/69521       | 0.81        | 28/108529 (0.0%) |
| 2   | B     | 0.26         | 0/2878        | 0.88        | 7/4490 (0.2%)    |
| 3   | C     | 0.51         | 0/2165        | 0.70        | 0/2919           |
| 4   | D     | 0.46         | 1/1601 (0.1%) | 0.73        | 3/2160 (0.1%)    |
| 5   | E     | 0.45         | 1/1620 (0.1%) | 0.64        | 1/2194 (0.0%)    |
| 6   | F     | 0.31         | 0/1499        | 0.57        | 1/2016 (0.0%)    |
| 7   | G     | 0.33         | 1/1332 (0.1%) | 0.73        | 2/1802 (0.1%)    |
| 8   | H     | 0.40         | 0/1151        | 0.75        | 1/1558 (0.1%)    |
| 9   | I     | 0.41         | 0/1131        | 0.62        | 0/1525           |
| 10  | J     | 0.41         | 0/943         | 0.62        | 1/1269 (0.1%)    |
| 11  | K     | 0.48         | 1/1162 (0.1%) | 0.83        | 1/1544 (0.1%)    |
| 12  | L     | 0.44         | 0/1143        | 0.71        | 1/1527 (0.1%)    |
| 13  | M     | 0.42         | 0/982         | 0.69        | 0/1312           |
| 14  | N     | 0.36         | 0/892         | 0.64        | 0/1187           |
| 15  | O     | 0.41         | 0/1155        | 0.63        | 0/1542           |
| 16  | P     | 0.40         | 0/982         | 0.65        | 0/1306           |
| 17  | Q     | 0.38         | 0/790         | 0.61        | 1/1057 (0.1%)    |
| 18  | R     | 0.50         | 0/911         | 0.67        | 0/1220           |
| 19  | S     | 0.47         | 0/739         | 0.62        | 0/993            |
| 20  | T     | 0.44         | 0/798         | 0.68        | 0/1064           |
| 21  | U     | 0.34         | 0/1493        | 0.60        | 0/2026           |
| 22  | V     | 0.45         | 0/657         | 0.65        | 0/874            |
| 23  | W     | 0.44         | 0/770         | 0.66        | 0/1022           |
| 24  | X     | 0.39         | 0/583         | 0.65        | 0/771            |
| 25  | Y     | 0.35         | 0/474         | 0.57        | 0/635            |
| 26  | Z     | 0.33         | 0/594         | 0.68        | 0/795            |
| 27  | a     | 0.43         | 0/473         | 0.78        | 0/639            |
| 28  | b     | 0.35         | 0/431         | 0.69        | 0/575            |
| 29  | c     | 0.49         | 0/438         | 0.68        | 0/575            |
| 30  | d     | 0.55         | 0/525         | 0.79        | 0/691            |
| 31  | e     | 0.26         | 0/310         | 0.45        | 0/407            |
| 32  | f     | 0.22         | 0/56          | 0.45        | 0/70             |

| Mol | Chain | Bond lengths |                 | Bond angles |                  |
|-----|-------|--------------|-----------------|-------------|------------------|
|     |       | RMSZ         | # Z  >5         | RMSZ        | # Z  >5          |
| All | All   | 0.31         | 4/100199 (0.0%) | 0.78        | 47/150294 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 7   | G     | 0                   | 1                   |
| 26  | Z     | 0                   | 1                   |
| 30  | d     | 0                   | 2                   |
| All | All   | 0                   | 4                   |

All (4) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 11  | K     | 10  | PRO  | N-CD  | 5.58 | 1.55        | 1.47     |
| 4   | D     | 22  | PRO  | N-CD  | 5.15 | 1.55        | 1.47     |
| 7   | G     | 128 | PRO  | N-CD  | 5.10 | 1.54        | 1.47     |
| 5   | E     | 25  | PRO  | N-CD  | 5.09 | 1.54        | 1.47     |

All (47) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|--------|-------------|----------|
| 7   | G     | 125  | VAL  | C-N-CD     | -17.76 | 81.53       | 120.60   |
| 12  | L     | 77   | LYS  | C-N-CD     | -8.42  | 102.08      | 120.60   |
| 2   | B     | 95   | U    | C5-C4-O4   | 7.82   | 130.59      | 125.90   |
| 1   | A     | 2506 | U    | C2-N1-C1'  | 7.42   | 126.61      | 117.70   |
| 1   | A     | 2702 | U    | C2-N1-C1'  | 6.85   | 125.92      | 117.70   |
| 2   | B     | 81   | G    | C5-C6-O6   | -6.84  | 124.50      | 128.60   |
| 1   | A     | 828  | U    | C2-N1-C1'  | 6.80   | 125.86      | 117.70   |
| 1   | A     | 673  | C    | C2-N3-C4   | -6.75  | 116.53      | 119.90   |
| 1   | A     | 828  | U    | N1-C2-O2   | 6.41   | 127.29      | 122.80   |
| 1   | A     | 807  | U    | C2-N3-C4   | -6.26  | 123.24      | 127.00   |
| 1   | A     | 828  | U    | N3-C2-O2   | -6.14  | 117.90      | 122.20   |
| 1   | A     | 2335 | A    | O4'-C1'-N9 | 6.00   | 113.00      | 108.20   |
| 1   | A     | 669  | G    | C4-N9-C1'  | 5.99   | 134.29      | 126.50   |
| 6   | F     | 34   | LEU  | CA-CB-CG   | 5.99   | 129.08      | 115.30   |
| 4   | D     | 63   | LEU  | CA-CB-CG   | 5.80   | 128.64      | 115.30   |
| 5   | E     | 24   | LEU  | C-N-CD     | 5.73   | 140.43      | 128.40   |
| 1   | A     | 2702 | U    | C5-C6-N1   | 5.68   | 125.54      | 122.70   |
| 7   | G     | 127  | GLU  | C-N-CD     | 5.67   | 140.31      | 128.40   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 2   | B     | 76   | G    | C6-N1-C2  | -5.65 | 121.71      | 125.10   |
| 4   | D     | 22   | PRO  | CA-N-CD   | -5.56 | 103.71      | 111.50   |
| 1   | A     | 103  | A    | N1-C6-N6  | 5.51  | 121.91      | 118.60   |
| 1   | A     | 2447 | G    | C6-N1-C2  | -5.50 | 121.80      | 125.10   |
| 4   | D     | 27   | LEU  | CA-CB-CG  | 5.46  | 127.87      | 115.30   |
| 11  | K     | 88   | LEU  | CA-CB-CG  | 5.46  | 127.85      | 115.30   |
| 1   | A     | 673  | C    | C5-C4-N4  | -5.37 | 116.44      | 120.20   |
| 2   | B     | 76   | G    | N3-C2-N2  | -5.35 | 116.16      | 119.90   |
| 1   | A     | 669  | G    | C8-N9-C1' | -5.34 | 120.06      | 127.00   |
| 1   | A     | 205  | G    | P-O3'-C3' | 5.33  | 126.10      | 119.70   |
| 1   | A     | 404  | C    | P-O3'-C3' | 5.33  | 126.10      | 119.70   |
| 2   | B     | 31   | C    | N1-C2-O2  | 5.29  | 122.07      | 118.90   |
| 2   | B     | 81   | G    | C6-N1-C2  | -5.23 | 121.96      | 125.10   |
| 1   | A     | 103  | A    | C4-C5-C6  | 5.22  | 119.61      | 117.00   |
| 10  | J     | 8    | LEU  | CA-CB-CG  | 5.21  | 127.28      | 115.30   |
| 1   | A     | 2506 | U    | C6-N1-C1' | -5.20 | 113.92      | 121.20   |
| 1   | A     | 2702 | U    | N1-C2-O2  | 5.17  | 126.42      | 122.80   |
| 2   | B     | 81   | G    | N3-C4-N9  | 5.17  | 129.10      | 126.00   |
| 1   | A     | 1312 | U    | P-O3'-C3' | 5.16  | 125.89      | 119.70   |
| 1   | A     | 1535 | U    | C2-N1-C1' | 5.15  | 123.88      | 117.70   |
| 1   | A     | 1799 | G    | P-O3'-C3' | 5.13  | 125.86      | 119.70   |
| 1   | A     | 1992 | G    | P-O3'-C3' | 5.12  | 125.85      | 119.70   |
| 1   | A     | 2726 | U    | C2-N1-C1' | 5.09  | 123.81      | 117.70   |
| 17  | Q     | 35   | LEU  | CA-CB-CG  | 5.09  | 127.00      | 115.30   |
| 1   | A     | 2506 | U    | N1-C2-O2  | 5.08  | 126.36      | 122.80   |
| 1   | A     | 537  | C    | C2-N1-C1' | 5.05  | 124.36      | 118.80   |
| 1   | A     | 242  | G    | P-O3'-C3' | 5.03  | 125.74      | 119.70   |
| 8   | H     | 74   | ASN  | N-CA-C    | 5.01  | 124.54      | 111.00   |
| 1   | A     | 222  | A    | P-O3'-C3' | 5.00  | 125.70      | 119.70   |

There are no chirality outliers.

All (4) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 7   | G     | 153 | LYS  | Peptide |
| 26  | Z     | 38  | LYS  | Peptide |
| 30  | d     | 30  | ARG  | Peptide |
| 30  | d     | 35  | GLN  | Peptide |

## 5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 62071 | 0        | 31284    | 714     | 0            |
| 2   | B     | 2573  | 0        | 1306     | 41      | 0            |
| 3   | C     | 2115  | 0        | 2195     | 95      | 0            |
| 4   | D     | 1568  | 0        | 1634     | 96      | 0            |
| 5   | E     | 1585  | 0        | 1632     | 86      | 0            |
| 6   | F     | 1474  | 0        | 1535     | 54      | 0            |
| 7   | G     | 1307  | 0        | 1382     | 74      | 0            |
| 8   | H     | 1136  | 0        | 1223     | 75      | 0            |
| 9   | I     | 1104  | 0        | 1180     | 41      | 0            |
| 10  | J     | 933   | 0        | 996      | 21      | 0            |
| 11  | K     | 1145  | 0        | 1226     | 78      | 0            |
| 12  | L     | 1122  | 0        | 1179     | 57      | 0            |
| 13  | M     | 968   | 0        | 1033     | 45      | 0            |
| 14  | N     | 882   | 0        | 943      | 42      | 0            |
| 15  | O     | 1141  | 0        | 1202     | 58      | 0            |
| 16  | P     | 964   | 0        | 1022     | 31      | 0            |
| 17  | Q     | 779   | 0        | 852      | 20      | 0            |
| 18  | R     | 900   | 0        | 964      | 23      | 0            |
| 19  | S     | 725   | 0        | 778      | 26      | 0            |
| 20  | T     | 785   | 0        | 878      | 48      | 0            |
| 21  | U     | 1461  | 0        | 1493     | 64      | 0            |
| 22  | V     | 648   | 0        | 672      | 20      | 0            |
| 23  | W     | 763   | 0        | 848      | 29      | 0            |
| 24  | X     | 581   | 0        | 629      | 15      | 0            |
| 25  | Y     | 469   | 0        | 518      | 6       | 0            |
| 26  | Z     | 581   | 0        | 574      | 23      | 0            |
| 27  | a     | 459   | 0        | 476      | 0       | 0            |
| 28  | b     | 424   | 0        | 450      | 0       | 0            |
| 29  | c     | 430   | 0        | 480      | 0       | 0            |
| 30  | d     | 517   | 0        | 582      | 0       | 0            |
| 31  | e     | 307   | 0        | 338      | 0       | 0            |
| 32  | f     | 116   | 0        | 67       | 0       | 0            |
| 33  | A     | 243   | 0        | 0        | 0       | 0            |
| 33  | B     | 2     | 0        | 0        | 0       | 0            |
| 33  | C     | 3     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 33  | D     | 2     | 0        | 0        | 0       | 0            |
| 33  | E     | 1     | 0        | 0        | 0       | 0            |
| 33  | K     | 3     | 0        | 0        | 0       | 0            |
| 33  | P     | 1     | 0        | 0        | 0       | 0            |
| 33  | V     | 1     | 0        | 0        | 0       | 0            |
| 34  | a     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 92290 | 0        | 61571    | 1669    | 0            |

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 12.

All (1669) close contacts within the same asymmetric unit are listed below.

| Atom-1           | Atom-2          | Distance(Å) | Clash(Å) |
|------------------|-----------------|-------------|----------|
| 7:G:125:VAL:HG12 | 7:G:126:PRO:CD  | 1.64        | 1.25     |
| 4:D:21:VAL:HG23  | 4:D:22:PRO:CB   | 1.69        | 1.22     |
| 7:G:125:VAL:CG1  | 7:G:126:PRO:HD3 | 1.75        | 1.16     |
| 1:A:1169:G:H1    | 1:A:1180:C:N4   | 1.48        | 1.09     |
| 4:D:21:VAL:HG23  | 4:D:22:PRO:HB3  | 1.18        | 1.09     |
| 4:D:21:VAL:CG2   | 4:D:22:PRO:HB3  | 1.87        | 1.05     |
| 8:H:52:ARG:O     | 8:H:56:LYS:N    | 1.91        | 1.02     |
| 7:G:125:VAL:HG12 | 7:G:126:PRO:HD3 | 1.01        | 0.99     |
| 1:A:1542:G:H3'   | 1:A:1543:A:C5'  | 1.92        | 0.99     |
| 1:A:1542:G:H3'   | 1:A:1543:A:H5'  | 1.43        | 0.96     |
| 1:A:2053:G:O6    | 1:A:2614:A:H2   | 1.49        | 0.96     |
| 4:D:20:ALA:O     | 4:D:21:VAL:HG13 | 1.65        | 0.95     |
| 4:D:13:ARG:HB2   | 4:D:21:VAL:HG12 | 1.47        | 0.95     |
| 8:H:57:ARG:O     | 8:H:61:ARG:HG2  | 1.67        | 0.93     |
| 1:A:2308:G:H1    | 1:A:2311:A:H2   | 1.15        | 0.93     |
| 4:D:21:VAL:HG23  | 4:D:22:PRO:CA   | 1.99        | 0.92     |
| 8:H:52:ARG:HB2   | 8:H:56:LYS:HB2  | 1.48        | 0.92     |
| 2:B:38:C:H42     | 2:B:44:G:H1     | 1.17        | 0.92     |
| 8:H:52:ARG:O     | 8:H:56:LYS:HB3  | 1.69        | 0.92     |
| 11:K:58:THR:O    | 11:K:61:ARG:NE  | 2.03        | 0.91     |
| 7:G:125:VAL:HG12 | 7:G:126:PRO:CG  | 1.98        | 0.91     |
| 1:A:1043:C:H42   | 1:A:1112:G:H1   | 0.97        | 0.91     |
| 1:A:2580:U:H4'   | 4:D:130:GLY:HA3 | 1.54        | 0.90     |
| 12:L:81:VAL:O    | 12:L:82:ARG:NE  | 2.05        | 0.89     |
| 8:H:54:GLN:O     | 8:H:58:LEU:HB2  | 1.73        | 0.89     |
| 1:A:2839:G:H5'   | 13:M:46:GLY:HA2 | 1.54        | 0.89     |
| 15:O:26:ASP:HB3  | 15:O:92:GLY:H   | 1.36        | 0.88     |
| 1:A:2287:A:N6    | 1:A:2344:U:H3   | 1.71        | 0.88     |
| 1:A:2701:C:H3'   | 1:A:2702:U:H5'' | 1.52        | 0.88     |

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| Atom-1            | Atom-2           | Distance(Å) | Clash(Å) |
|-------------------|------------------|-------------|----------|
| 5:E:6:VAL:HB      | 5:E:24:LEU:HB2   | 1.57        | 0.87     |
| 4:D:13:ARG:HB2    | 4:D:21:VAL:CG1   | 2.03        | 0.87     |
| 11:K:64:LYS:O     | 11:K:66:GLY:N    | 2.07        | 0.87     |
| 1:A:1543:A:H1'    | 1:A:1545:A:O4'   | 1.75        | 0.87     |
| 1:A:2287:A:H62    | 1:A:2344:U:H3    | 0.90        | 0.86     |
| 11:K:19:VAL:HG13  | 11:K:21:ARG:H    | 1.40        | 0.86     |
| 1:A:1169:G:N2     | 1:A:1180:C:N3    | 2.23        | 0.86     |
| 1:A:847:U:O4      | 1:A:933:A:N1     | 2.08        | 0.86     |
| 21:U:111:VAL:HG22 | 21:U:112:ARG:H   | 1.39        | 0.86     |
| 3:C:43:ARG:NH1    | 3:C:44:ASN:OD1   | 2.09        | 0.85     |
| 8:H:53:ALA:O      | 8:H:57:ARG:HG3   | 1.77        | 0.85     |
| 1:A:806:C:OP2     | 11:K:41:ARG:NH1  | 2.09        | 0.85     |
| 20:T:79:CYS:SG    | 20:T:80:GLY:N    | 2.45        | 0.84     |
| 1:A:1043:C:N3     | 1:A:1112:G:N2    | 2.25        | 0.84     |
| 2:B:33:G:H5'      | 6:F:2:PRO:HG3    | 1.59        | 0.84     |
| 1:A:49:A:N7       | 1:A:120:U:C4     | 2.45        | 0.84     |
| 8:H:52:ARG:HB2    | 8:H:56:LYS:CB    | 2.08        | 0.84     |
| 1:A:1043:C:N4     | 1:A:1112:G:H1    | 1.74        | 0.84     |
| 1:A:1359:A:N1     | 1:A:1372:U:O4    | 2.11        | 0.83     |
| 1:A:857:C:H4'     | 22:V:23:VAL:HG21 | 1.59        | 0.83     |
| 1:A:530:G:O2'     | 1:A:532:A:N7     | 2.12        | 0.82     |
| 8:H:55:ALA:O      | 8:H:58:LEU:HB3   | 1.78        | 0.82     |
| 4:D:20:ALA:C      | 4:D:21:VAL:HG13  | 1.97        | 0.82     |
| 5:E:197:ASP:O     | 5:E:199:TRP:N    | 2.12        | 0.82     |
| 20:T:29:GLU:HB3   | 20:T:38:ILE:HG12 | 1.62        | 0.82     |
| 4:D:22:PRO:HD2    | 4:D:185:LYS:HD2  | 1.61        | 0.81     |
| 1:A:2308:G:N1     | 1:A:2311:A:C2    | 2.47        | 0.81     |
| 1:A:2068:U:H3     | 1:A:2430:A:H2    | 1.28        | 0.81     |
| 4:D:15:PHE:CD1    | 4:D:20:ALA:HB2   | 2.14        | 0.81     |
| 5:E:103:LYS:HA    | 5:E:106:ARG:HG3  | 1.63        | 0.81     |
| 24:X:47:ASN:O     | 24:X:49:LYS:N    | 2.13        | 0.81     |
| 4:D:201:THR:HG22  | 4:D:203:LYS:H    | 1.45        | 0.81     |
| 15:O:24:PRO:HA    | 15:O:49:VAL:HG13 | 1.61        | 0.80     |
| 1:A:676:A:H8      | 1:A:2069:G:H21   | 1.29        | 0.80     |
| 1:A:273:G:H1      | 1:A:364:C:H42    | 1.27        | 0.80     |
| 21:U:108:PRO:HA   | 21:U:142:SER:HA  | 1.60        | 0.80     |
| 4:D:50:GLY:HA2    | 4:D:77:ILE:HA    | 1.64        | 0.80     |
| 9:I:42:TRP:O      | 16:P:64:ARG:NH2  | 2.15        | 0.80     |
| 1:A:847:U:C4      | 1:A:933:A:N1     | 2.50        | 0.80     |
| 1:A:958:U:OP2     | 12:L:14:ARG:NH1  | 2.13        | 0.80     |
| 1:A:270(R):G:N3   | 23:W:78:LYS:NZ   | 2.30        | 0.80     |
| 1:A:768:G:O2'     | 1:A:1379:A:N6    | 2.14        | 0.80     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:A:2445:G:OP1    | 5:E:74:ARG:NH2    | 2.15        | 0.80     |
| 13:M:104:ARG:HD2  | 13:M:111:LEU:HD21 | 1.63        | 0.79     |
| 1:A:978:G:H1      | 1:A:985:C:H42     | 1.28        | 0.79     |
| 1:A:270(T):G:H5'' | 23:W:97:LEU:HD22  | 1.65        | 0.78     |
| 1:A:1048:A:H2     | 1:A:1112:G:H21    | 1.32        | 0.78     |
| 21:U:108:PRO:HG2  | 21:U:110:GLY:O    | 1.84        | 0.78     |
| 11:K:126:VAL:HG12 | 11:K:147:LEU:HD21 | 1.63        | 0.78     |
| 9:I:95:PRO:O      | 9:I:97:ARG:N      | 2.15        | 0.78     |
| 3:C:69:ARG:NH2    | 3:C:128:GLY:O     | 2.17        | 0.78     |
| 1:A:1359:A:C6     | 1:A:1372:U:O4     | 2.37        | 0.78     |
| 8:H:4:ILE:HD11    | 8:H:44:LEU:HD12   | 1.66        | 0.77     |
| 1:A:2308:G:N1     | 1:A:2311:A:H2     | 1.82        | 0.77     |
| 1:A:1311:G:N2     | 1:A:1603:A:H62    | 1.83        | 0.77     |
| 1:A:590:A:OP1     | 5:E:95:ARG:NH1    | 2.17        | 0.77     |
| 1:A:2807:G:N1     | 1:A:2893:G:O6     | 2.17        | 0.77     |
| 5:E:66:PRO:O      | 5:E:68:LYS:N      | 2.18        | 0.77     |
| 1:A:1021:A:H61    | 1:A:1142(A):A:H61 | 1.29        | 0.77     |
| 15:O:41:ARG:HB2   | 15:O:41:ARG:NH1   | 1.99        | 0.77     |
| 1:A:873:G:H1      | 1:A:904:C:H42     | 1.31        | 0.77     |
| 7:G:125:VAL:CG1   | 7:G:126:PRO:CG    | 2.63        | 0.77     |
| 4:D:9:VAL:HB      | 4:D:25:VAL:HG23   | 1.66        | 0.76     |
| 13:M:3:HIS:O      | 13:M:5:LYS:N      | 2.19        | 0.76     |
| 2:B:40:U:O2       | 2:B:45:A:N6       | 2.19        | 0.76     |
| 14:N:62:LYS:HB3   | 14:N:97:ARG:HD3   | 1.67        | 0.76     |
| 4:D:15:PHE:CE1    | 4:D:20:ALA:HB2    | 2.21        | 0.75     |
| 20:T:95:LYS:HB3   | 20:T:100:ALA:HA   | 1.68        | 0.75     |
| 1:A:1071:G:O6     | 1:A:1091:G:O6     | 2.03        | 0.75     |
| 20:T:87:LYS:HD3   | 20:T:92:ASN:HB3   | 1.69        | 0.75     |
| 13:M:74:LYS:O     | 13:M:76:VAL:N     | 2.18        | 0.75     |
| 11:K:14:LYS:O     | 11:K:16:ARG:N     | 2.20        | 0.75     |
| 20:T:86:ARG:HB2   | 20:T:95:LYS:HD2   | 1.69        | 0.75     |
| 1:A:155:C:H42     | 1:A:171:G:H1      | 1.35        | 0.74     |
| 13:M:56:LYS:NZ    | 13:M:90:ARG:O     | 2.20        | 0.74     |
| 1:A:674:G:H1'     | 5:E:74:ARG:HD3    | 1.69        | 0.74     |
| 6:F:34:LEU:HB2    | 6:F:172:LEU:HD21  | 1.68        | 0.74     |
| 21:U:60:GLU:HA    | 21:U:66:SER:HA    | 1.68        | 0.74     |
| 5:E:6:VAL:HB      | 5:E:24:LEU:CB     | 2.18        | 0.74     |
| 4:D:62:PRO:O      | 4:D:64:LYS:N      | 2.20        | 0.74     |
| 1:A:1693:U:O2'    | 3:C:14:ARG:NH2    | 2.21        | 0.73     |
| 23:W:7:ILE:HG12   | 23:W:91:LYS:HZ1   | 1.51        | 0.73     |
| 1:A:1443:G:H1     | 1:A:1548:C:H42    | 1.35        | 0.73     |
| 1:A:1071:G:N1     | 1:A:1091:G:N7     | 2.33        | 0.73     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 21:U:111:VAL:HG22 | 21:U:112:ARG:N    | 2.03        | 0.73     |
| 1:A:1019:U:H3     | 1:A:1142(A):A:H62 | 1.37        | 0.72     |
| 1:A:1607:C:N4     | 1:A:1622:G:OP2    | 2.22        | 0.72     |
| 1:A:392:C:H5''    | 1:A:409:C:H5''    | 1.70        | 0.72     |
| 1:A:1411:C:H42    | 1:A:1591:G:H1     | 1.34        | 0.72     |
| 1:A:882:G:H1      | 1:A:894:C:H42     | 1.35        | 0.72     |
| 8:H:5:LEU:HD11    | 8:H:19:VAL:HG12   | 1.70        | 0.72     |
| 1:A:2502:G:H5''   | 1:A:2503:A:H5''   | 1.70        | 0.72     |
| 4:D:21:VAL:HG23   | 4:D:22:PRO:N      | 2.05        | 0.72     |
| 1:A:884:C:O2      | 1:A:892:G:N1      | 2.23        | 0.72     |
| 7:G:125:VAL:CG1   | 7:G:126:PRO:HG3   | 2.20        | 0.72     |
| 8:H:93:THR:HG22   | 8:H:119:PRO:HB3   | 1.72        | 0.72     |
| 7:G:125:VAL:HG12  | 7:G:126:PRO:HG3   | 1.70        | 0.72     |
| 22:V:68:GLU:OE1   | 22:V:82:ARG:NH1   | 2.23        | 0.71     |
| 1:A:987:G:O2'     | 1:A:1000:A:N3     | 2.20        | 0.71     |
| 1:A:1138:G:H21    | 9:I:106:MET:HE3   | 1.54        | 0.71     |
| 12:L:81:VAL:C     | 12:L:82:ARG:HG2   | 2.10        | 0.71     |
| 21:U:166:SER:HB2  | 21:U:168:GLU:N    | 2.05        | 0.71     |
| 5:E:24:LEU:HG     | 5:E:115:ALA:HB2   | 1.72        | 0.71     |
| 11:K:38:GLN:HG2   | 11:K:45:LEU:HD12  | 1.72        | 0.71     |
| 25:Y:8:LEU:HD13   | 25:Y:31:LEU:HD23  | 1.71        | 0.71     |
| 6:F:61:ALA:HB2    | 6:F:68:PRO:HD3    | 1.72        | 0.71     |
| 1:A:1045:A:C8     | 1:A:1111:A:N6     | 2.59        | 0.71     |
| 24:X:29:LYS:HE3   | 24:X:57:ILE:HG21  | 1.73        | 0.70     |
| 7:G:106:THR:HG22  | 7:G:112:PRO:HB3   | 1.72        | 0.70     |
| 8:H:98:ALA:HB2    | 8:H:111:PRO:HB3   | 1.72        | 0.70     |
| 1:A:1543:A:H1'    | 1:A:1545:A:C4'    | 2.21        | 0.70     |
| 18:R:29:LEU:HD22  | 18:R:69:LEU:HD11  | 1.72        | 0.70     |
| 1:A:1061:U:H5'    | 1:A:1070:A:H1'    | 1.74        | 0.70     |
| 15:O:18:ASP:N     | 15:O:18:ASP:OD1   | 2.20        | 0.70     |
| 1:A:1543:A:O2'    | 1:A:1544:C:H3'    | 1.90        | 0.70     |
| 8:H:52:ARG:O      | 8:H:56:LYS:CB     | 2.39        | 0.70     |
| 7:G:125:VAL:CG1   | 7:G:126:PRO:CD    | 2.48        | 0.70     |
| 1:A:265:A:N6      | 1:A:427:U:O2'     | 2.25        | 0.69     |
| 4:D:119:ARG:HB3   | 4:D:120:TRP:CD1   | 2.27        | 0.69     |
| 1:A:2404:C:O3'    | 11:K:77:ARG:NH2   | 2.24        | 0.69     |
| 3:C:93:ALA:HB3    | 3:C:105:ILE:HG22  | 1.74        | 0.69     |
| 26:Z:18:CYS:SG    | 26:Z:19:GLY:N     | 2.65        | 0.69     |
| 2:B:38:C:N4       | 2:B:44:G:H1       | 1.90        | 0.69     |
| 26:Z:7:PRO:HB2    | 26:Z:27:THR:HG21  | 1.74        | 0.69     |
| 12:L:37:LEU:HD21  | 12:L:130:LYS:HE3  | 1.74        | 0.69     |
| 7:G:86:GLU:HG3    | 7:G:165:ALA:H     | 1.56        | 0.69     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:2857:G:N2    | 1:A:2860:A:OP2   | 2.22        | 0.69     |
| 1:A:1045:A:C6    | 1:A:1111:A:N7    | 2.61        | 0.68     |
| 1:A:2287:A:N6    | 1:A:2344:U:N3    | 2.35        | 0.68     |
| 4:D:2:LYS:HD3    | 4:D:95:ILE:HG22  | 1.75        | 0.68     |
| 8:H:52:ARG:C     | 8:H:56:LYS:HB3   | 2.12        | 0.68     |
| 18:R:29:LEU:HG   | 18:R:33:ARG:HD2  | 1.74        | 0.68     |
| 3:C:25:THR:O     | 3:C:27:THR:N     | 2.26        | 0.68     |
| 21:U:110:GLY:HA2 | 21:U:111:VAL:C   | 2.14        | 0.68     |
| 1:A:273:G:H1     | 1:A:364:C:N4     | 1.90        | 0.68     |
| 6:F:66:GLN:NE2   | 6:F:93:THR:O     | 2.26        | 0.68     |
| 6:F:47:LYS:HD3   | 6:F:81:LYS:HB2   | 1.76        | 0.68     |
| 1:A:2131:G:H4'   | 1:A:2132:U:H4'   | 1.74        | 0.68     |
| 13:M:38:VAL:HG22 | 13:M:112:ALA:HB2 | 1.75        | 0.68     |
| 1:A:1689:A:H62   | 1:A:1698:A:H2    | 1.42        | 0.68     |
| 1:A:654(A):G:H1  | 1:A:654(T):C:N4  | 1.91        | 0.68     |
| 1:A:978:G:H1     | 1:A:985:C:N4     | 1.92        | 0.68     |
| 12:L:12:GLN:HG2  | 12:L:73:PRO:HD2  | 1.75        | 0.68     |
| 6:F:83:ARG:H     | 6:F:86:MET:HG3   | 1.59        | 0.67     |
| 1:A:2115:G:N2    | 1:A:2165:G:N7    | 2.36        | 0.67     |
| 7:G:127:GLU:HB2  | 7:G:130:ARG:HB3  | 1.76        | 0.67     |
| 7:G:152:ARG:HG3  | 7:G:153:LYS:HD2  | 1.77        | 0.67     |
| 1:A:587:C:OP2    | 11:K:21:ARG:NH2  | 2.28        | 0.67     |
| 4:D:20:ALA:C     | 4:D:21:VAL:CG1   | 2.62        | 0.67     |
| 1:A:1187:G:H5''  | 17:Q:81:TYR:CE1  | 2.29        | 0.67     |
| 17:Q:72:VAL:HG13 | 17:Q:85:LYS:HB3  | 1.75        | 0.67     |
| 1:A:2168:G:N2    | 1:A:2170:A:N7    | 2.38        | 0.67     |
| 1:A:807:U:H2'    | 1:A:808:G:H8     | 1.60        | 0.67     |
| 3:C:182:LEU:H    | 3:C:272:ALA:HB3  | 1.59        | 0.67     |
| 1:A:857:C:OP2    | 22:V:77:ARG:NH2  | 2.23        | 0.67     |
| 15:O:84:GLN:HG2  | 15:O:85:LYS:HG2  | 1.76        | 0.67     |
| 1:A:49:A:N7      | 1:A:120:U:C5     | 2.63        | 0.67     |
| 5:E:143:ALA:HB1  | 5:E:148:LEU:HB2  | 1.75        | 0.67     |
| 7:G:41:MET:HE1   | 7:G:64:LEU:HD22  | 1.75        | 0.67     |
| 1:A:598:G:H5'    | 11:K:11:GLY:HA3  | 1.77        | 0.67     |
| 3:C:49:ILE:HD11  | 3:C:52:ARG:HA    | 1.77        | 0.67     |
| 1:A:2392:A:C8    | 11:K:60:MET:HG2  | 2.30        | 0.67     |
| 15:O:36:GLU:HG3  | 15:O:41:ARG:HD3  | 1.77        | 0.67     |
| 8:H:3:VAL:HG12   | 8:H:38:LEU:HA    | 1.77        | 0.66     |
| 12:L:30:GLY:HA2  | 12:L:107:ALA:HB2 | 1.78        | 0.66     |
| 1:A:654(A):G:N2  | 1:A:654(T):C:N3  | 2.44        | 0.66     |
| 8:H:4:ILE:HG12   | 8:H:18:VAL:HG22  | 1.78        | 0.66     |
| 1:A:270(R):G:OP1 | 8:H:42:SER:OG    | 2.12        | 0.66     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 2:B:24:G:O6       | 2:B:56:G:O2'      | 2.12        | 0.66     |
| 1:A:2392:A:H8     | 11:K:60:MET:HG2   | 1.59        | 0.66     |
| 6:F:6:ALA:H       | 26:Z:23:GLU:HG2   | 1.60        | 0.66     |
| 23:W:7:ILE:HG12   | 23:W:91:LYS:NZ    | 2.11        | 0.66     |
| 1:A:2298:A:H62    | 1:A:2318:G:H8     | 1.44        | 0.66     |
| 1:A:372:G:N2      | 1:A:401:A:OP2     | 2.23        | 0.66     |
| 4:D:63:LEU:HD13   | 4:D:65:GLY:H      | 1.60        | 0.66     |
| 5:E:149:ASP:OD1   | 5:E:149:ASP:N     | 2.27        | 0.66     |
| 12:L:135:ASP:OD1  | 12:L:135:ASP:N    | 2.23        | 0.66     |
| 20:T:49:VAL:O     | 20:T:51:VAL:N     | 2.29        | 0.66     |
| 21:U:19:ARG:NH1   | 21:U:84:GLU:O     | 2.28        | 0.66     |
| 15:O:102:ILE:HB   | 15:O:110:ILE:HD13 | 1.78        | 0.65     |
| 1:A:1359:A:N1     | 1:A:1372:U:C4     | 2.64        | 0.65     |
| 1:A:2747:G:H21    | 1:A:2757:A:H62    | 1.43        | 0.65     |
| 26:Z:1:MET:SD     | 26:Z:6:HIS:NE2    | 2.69        | 0.65     |
| 3:C:108:PRO:HG2   | 3:C:111:LEU:HG    | 1.78        | 0.65     |
| 3:C:27:THR:HG21   | 3:C:81:ALA:HB1    | 1.78        | 0.65     |
| 7:G:125:VAL:CB    | 7:G:126:PRO:HD3   | 2.16        | 0.65     |
| 7:G:89:ILE:CD1    | 7:G:129:THR:HB    | 2.27        | 0.65     |
| 1:A:483:A:H4'     | 20:T:49:VAL:HA    | 1.78        | 0.65     |
| 11:K:59:LEU:HA    | 11:K:61:ARG:NE    | 2.12        | 0.65     |
| 21:U:150:LEU:HD21 | 21:U:172:ALA:HB3  | 1.77        | 0.65     |
| 1:A:224:G:O6      | 1:A:419:C:O2'     | 2.15        | 0.65     |
| 20:T:38:ILE:HG22  | 20:T:66:PRO:HA    | 1.79        | 0.65     |
| 1:A:27:G:N2       | 1:A:513:A:OP2     | 2.29        | 0.65     |
| 1:A:504:U:H5''    | 1:A:505:A:H5'     | 1.78        | 0.65     |
| 4:D:14:ILE:O      | 4:D:21:VAL:N      | 2.28        | 0.65     |
| 11:K:71:VAL:HG13  | 11:K:72:PRO:HD3   | 1.78        | 0.65     |
| 11:K:47:ASP:OD2   | 11:K:50:ARG:NH2   | 2.30        | 0.65     |
| 1:A:2701:C:H3'    | 1:A:2702:U:C5'    | 2.23        | 0.65     |
| 1:A:819:A:OP2     | 1:A:1187:G:N2     | 2.24        | 0.65     |
| 5:E:31:HIS:HB2    | 11:K:9:ASN:OD1    | 1.96        | 0.65     |
| 10:J:4:PRO:O      | 10:J:5:GLN:HB2    | 1.96        | 0.64     |
| 1:A:2693:A:H2'    | 1:A:2694:G:H8     | 1.62        | 0.64     |
| 3:C:35:LYS:HG2    | 3:C:64:ILE:N      | 2.12        | 0.64     |
| 11:K:85:LEU:HA    | 11:K:88:LEU:HD22  | 1.79        | 0.64     |
| 1:A:2683:C:OP1    | 15:O:53:ARG:NH2   | 2.30        | 0.64     |
| 1:A:489:G:N7      | 18:R:49:LYS:NZ    | 2.46        | 0.64     |
| 3:C:8:PRO:HB3     | 3:C:14:ARG:HB2    | 1.79        | 0.64     |
| 3:C:65:ILE:HD11   | 3:C:67:PHE:CE2    | 2.31        | 0.64     |
| 4:D:21:VAL:CB     | 4:D:22:PRO:HA     | 2.28        | 0.64     |
| 1:A:141:A:H8      | 1:A:1595:G:H21    | 1.46        | 0.64     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:A:2114:A:N6     | 1:A:2119:A:N7     | 2.46        | 0.64     |
| 12:L:17:LEU:HD21  | 12:L:41:TRP:CD1   | 2.33        | 0.64     |
| 16:P:90:VAL:O     | 16:P:92:ARG:N     | 2.30        | 0.64     |
| 1:A:2636:U:OP1    | 4:D:79:ARG:HA     | 1.97        | 0.64     |
| 3:C:35:LYS:HG2    | 3:C:64:ILE:H      | 1.63        | 0.64     |
| 1:A:1543:A:C2     | 1:A:1545:A:C8     | 2.86        | 0.64     |
| 1:A:2100:G:H1     | 1:A:2189:U:H3     | 1.44        | 0.64     |
| 1:A:2547:U:O2     | 10:J:23:ARG:NH2   | 2.31        | 0.64     |
| 5:E:192:LEU:HD22  | 5:E:194:MET:HG2   | 1.80        | 0.64     |
| 7:G:88:LEU:HD11   | 7:G:165:ALA:HB2   | 1.80        | 0.64     |
| 11:K:10:PRO:O     | 11:K:12:ALA:N     | 2.30        | 0.64     |
| 12:L:83:MET:HB2   | 22:V:7:LEU:HD12   | 1.78        | 0.64     |
| 26:Z:48:ARG:O     | 26:Z:50:VAL:N     | 2.31        | 0.64     |
| 1:A:1059:G:O6     | 1:A:1079:C:N4     | 2.30        | 0.63     |
| 14:N:26:LEU:HB3   | 14:N:87:PHE:HA    | 1.81        | 0.63     |
| 19:S:43:VAL:HG13  | 19:S:51:VAL:HG21  | 1.79        | 0.63     |
| 1:A:1266:G:O2'    | 1:A:2012:G:O6     | 2.14        | 0.63     |
| 1:A:2848:G:O2'    | 1:A:2867:G:N2     | 2.31        | 0.63     |
| 13:M:104:ARG:HD3  | 13:M:109:ALA:HB3  | 1.79        | 0.63     |
| 1:A:2053:G:O6     | 1:A:2614:A:C2     | 2.41        | 0.63     |
| 4:D:21:VAL:CG2    | 4:D:22:PRO:CA     | 2.76        | 0.63     |
| 1:A:2849:U:OP1    | 15:O:95:ARG:NH1   | 2.30        | 0.63     |
| 21:U:165:VAL:HG11 | 21:U:169:GLU:HB2  | 1.80        | 0.63     |
| 23:W:29:GLY:O     | 23:W:31:GLY:N     | 2.29        | 0.63     |
| 1:A:2511:U:O4     | 1:A:2575:C:N3     | 2.32        | 0.63     |
| 1:A:309:G:N3      | 1:A:329:G:O2'     | 2.31        | 0.63     |
| 13:M:33:ARG:HG3   | 13:M:115:GLU:HB3  | 1.79        | 0.63     |
| 16:P:66:ASN:O     | 16:P:70:ARG:HB2   | 1.98        | 0.63     |
| 24:X:65:ASN:HB3   | 24:X:69:ARG:HH22  | 1.61        | 0.63     |
| 1:A:2224:G:OP1    | 3:C:268:ARG:HD3   | 1.98        | 0.63     |
| 11:K:95:VAL:HG13  | 11:K:100:LEU:HD21 | 1.79        | 0.63     |
| 1:A:2233:U:H2'    | 1:A:2234:G:C8     | 2.33        | 0.63     |
| 1:A:288:C:H2'     | 1:A:289:A:H8      | 1.64        | 0.63     |
| 1:A:74:A:H4'      | 1:A:75:G:O5'      | 1.98        | 0.63     |
| 1:A:84:A:N1       | 1:A:98:G:O2'      | 2.31        | 0.63     |
| 9:I:133:GLN:HB2   | 9:I:135:PRO:HD3   | 1.79        | 0.63     |
| 14:N:15:ARG:HH11  | 14:N:25:ARG:HH21  | 1.44        | 0.63     |
| 9:I:13:TRP:HB2    | 9:I:133:GLN:HG3   | 1.81        | 0.63     |
| 1:A:2818:G:OP2    | 13:M:42:LYS:NZ    | 2.31        | 0.63     |
| 20:T:51:VAL:HG13  | 20:T:52:SER:H     | 1.64        | 0.63     |
| 1:A:1311:G:H21    | 1:A:1603:A:H62    | 1.45        | 0.62     |
| 1:A:2306:C:H3'    | 1:A:2307:G:H5''   | 1.79        | 0.62     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 4:D:15:PHE:CE1   | 4:D:20:ALA:CB    | 2.82        | 0.62     |
| 1:A:1496:A:H8    | 1:A:1577:C:HO2'  | 1.47        | 0.62     |
| 1:A:2576:G:O2'   | 1:A:2579:C:OP2   | 2.16        | 0.62     |
| 1:A:27:G:H1'     | 1:A:513:A:N6     | 2.14        | 0.62     |
| 4:D:119:ARG:HG2  | 4:D:160:TYR:HB2  | 1.81        | 0.62     |
| 5:E:12:LEU:HD12  | 5:E:17:ARG:HG2   | 1.80        | 0.62     |
| 19:S:53:LYS:HB2  | 19:S:82:GLN:HB3  | 1.80        | 0.62     |
| 1:A:2816:C:O3'   | 13:M:99:LYS:NZ   | 2.33        | 0.62     |
| 1:A:2111:C:N3    | 1:A:2118:U:O2'   | 2.31        | 0.62     |
| 1:A:2133:G:H1'   | 1:A:2158:A:H61   | 1.64        | 0.62     |
| 2:B:44:G:O2'     | 2:B:47:C:N4      | 2.31        | 0.62     |
| 1:A:996:A:H4'    | 16:P:92:ARG:HE   | 1.64        | 0.62     |
| 15:O:54:ARG:HA   | 15:O:59:THR:HG23 | 1.82        | 0.62     |
| 1:A:221:A:H4'    | 1:A:222:A:O5'    | 1.98        | 0.62     |
| 3:C:35:LYS:HD2   | 3:C:104:TYR:CD1  | 2.35        | 0.62     |
| 1:A:630:G:N2     | 1:A:633:A:OP2    | 2.32        | 0.61     |
| 4:D:67:PHE:O     | 4:D:69:LYS:N     | 2.32        | 0.61     |
| 8:H:104:GLN:O    | 8:H:105:HIS:ND1  | 2.33        | 0.61     |
| 8:H:57:ARG:HA    | 8:H:60:GLU:HB3   | 1.81        | 0.61     |
| 1:A:1272:A:OP2   | 1:A:1647:G:OP1   | 2.18        | 0.61     |
| 1:A:2011:U:OP2   | 18:R:16:LYS:NZ   | 2.30        | 0.61     |
| 4:D:51:PHE:CD2   | 4:D:52:LEU:HG    | 2.34        | 0.61     |
| 5:E:28:ILE:HG22  | 5:E:112:MET:HB3  | 1.80        | 0.61     |
| 1:A:2405:G:O2'   | 1:A:2411:A:N6    | 2.33        | 0.61     |
| 1:A:884:C:N3     | 1:A:892:G:O6     | 2.33        | 0.61     |
| 21:U:166:SER:HB2 | 21:U:168:GLU:H   | 1.64        | 0.61     |
| 23:W:53:VAL:HG22 | 23:W:74:VAL:HG13 | 1.83        | 0.61     |
| 1:A:997:G:OP1    | 16:P:93:LYS:HD3  | 2.00        | 0.61     |
| 1:A:2444:G:OP2   | 5:E:68:LYS:HE3   | 2.00        | 0.61     |
| 8:H:5:LEU:HD13   | 8:H:17:GLN:HB3   | 1.81        | 0.61     |
| 11:K:84:ASN:HB3  | 11:K:86:LYS:HG2  | 1.83        | 0.61     |
| 12:L:65:PHE:O    | 12:L:67:ARG:N    | 2.34        | 0.61     |
| 18:R:25:ARG:NH2  | 18:R:74:ALA:O    | 2.33        | 0.61     |
| 1:A:468:G:H4'    | 5:E:62:ARG:HH12  | 1.65        | 0.61     |
| 1:A:856:C:O2'    | 1:A:857:C:OP1    | 2.16        | 0.61     |
| 1:A:1798:U:H5'   | 3:C:259:THR:HG22 | 1.83        | 0.61     |
| 7:G:8:PRO:HG2    | 7:G:69:ARG:HE    | 1.66        | 0.61     |
| 1:A:2712:U:HO2'  | 1:A:2712(A):A:H8 | 1.47        | 0.60     |
| 1:A:910:A:C5     | 12:L:13:GLN:HG3  | 2.36        | 0.60     |
| 13:M:70:LEU:O    | 13:M:72:ASP:N    | 2.31        | 0.60     |
| 1:A:994:C:OP2    | 16:P:54:LYS:NZ   | 2.34        | 0.60     |
| 15:O:77:PRO:HB2  | 15:O:80:SER:HB2  | 1.83        | 0.60     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 16:P:90:VAL:HG11  | 17:Q:40:LEU:HD12  | 1.82        | 0.60     |
| 1:A:1296:G:OP1    | 1:A:2709:G:O2'    | 2.11        | 0.60     |
| 1:A:155:C:N4      | 1:A:171:G:H1      | 1.99        | 0.60     |
| 1:A:873:G:H1      | 1:A:904:C:N4      | 1.98        | 0.60     |
| 3:C:44:ASN:HB3    | 3:C:49:ILE:HA     | 1.83        | 0.60     |
| 1:A:2443:C:H2'    | 1:A:2444:G:H8     | 1.66        | 0.60     |
| 1:A:1782:C:H1'    | 1:A:2609:U:H5''   | 1.82        | 0.60     |
| 3:C:70:TRP:CH2    | 3:C:150:LYS:HA    | 2.36        | 0.60     |
| 1:A:252:G:OP2     | 11:K:50:ARG:NH1   | 2.33        | 0.60     |
| 14:N:88:ASP:O     | 14:N:89:ARG:HB3   | 2.02        | 0.60     |
| 1:A:993:G:OP1     | 16:P:50:ARG:NH2   | 2.34        | 0.60     |
| 1:A:1169:G:H1     | 1:A:1180:C:H42    | 0.70        | 0.60     |
| 26:Z:23:GLU:O     | 26:Z:25:TYR:N     | 2.33        | 0.60     |
| 20:T:87:LYS:O     | 20:T:88:LYS:NZ    | 2.33        | 0.60     |
| 1:A:49:A:N7       | 1:A:120:U:O4      | 2.33        | 0.60     |
| 2:B:31:C:H42      | 2:B:51:G:H1       | 1.50        | 0.60     |
| 6:F:114:ILE:HD13  | 6:F:140:ILE:HG21  | 1.83        | 0.60     |
| 7:G:154:PRO:HD3   | 7:G:162:ILE:N     | 2.16        | 0.60     |
| 15:O:105:LEU:O    | 15:O:107:ASP:N    | 2.35        | 0.59     |
| 21:U:144:LEU:HG   | 21:U:150:LEU:HD12 | 1.84        | 0.59     |
| 7:G:89:ILE:HD13   | 7:G:129:THR:HB    | 1.83        | 0.59     |
| 6:F:64:THR:HG23   | 6:F:66:GLN:H      | 1.66        | 0.59     |
| 14:N:38:GLN:OE1   | 14:N:47:THR:OG1   | 2.18        | 0.59     |
| 21:U:52:SER:O     | 21:U:52:SER:OG    | 2.12        | 0.59     |
| 21:U:87:ASP:OD1   | 21:U:87:ASP:N     | 2.34        | 0.59     |
| 1:A:1291:C:H5'    | 1:A:1536:A:H5'    | 1.85        | 0.59     |
| 6:F:67:LYS:HE2    | 26:Z:6:HIS:CE1    | 2.38        | 0.59     |
| 1:A:1026:U:H4'    | 1:A:1027:A:OP1    | 2.02        | 0.59     |
| 1:A:83:G:N2       | 1:A:103:A:OP2     | 2.31        | 0.59     |
| 18:R:86:LEU:HD12  | 18:R:87:PRO:HD2   | 1.85        | 0.59     |
| 1:A:577:G:O2'     | 1:A:1254:A:OP1    | 2.18        | 0.59     |
| 4:D:21:VAL:HB     | 4:D:22:PRO:HA     | 1.85        | 0.59     |
| 7:G:121:ILE:HG13  | 7:G:140:LYS:HD2   | 1.84        | 0.59     |
| 1:A:1359:A:N6     | 1:A:1372:U:C5     | 2.70        | 0.59     |
| 1:A:1636:C:H2'    | 1:A:1637:A:C8     | 2.38        | 0.59     |
| 2:B:50:G:H5''     | 14:N:61:ASN:HD21  | 1.67        | 0.59     |
| 7:G:105:LEU:H     | 7:G:105:LEU:HD13  | 1.68        | 0.59     |
| 12:L:109:VAL:HG12 | 12:L:114:ALA:HB2  | 1.84        | 0.59     |
| 1:A:2010:G:H5''   | 18:R:42:ARG:HB2   | 1.85        | 0.59     |
| 3:C:85:ASP:HB2    | 3:C:92:ILE:HD13   | 1.84        | 0.59     |
| 23:W:92:LYS:HG3   | 23:W:96:LYS:HB2   | 1.84        | 0.59     |
| 26:Z:16:CYS:SG    | 26:Z:17:GLY:N     | 2.75        | 0.59     |

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| Atom-1           | Atom-2            | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:A:617:G:OP1    | 5:E:40:GLN:NE2    | 2.26        | 0.58     |
| 1:A:1918:A:O2'   | 1:A:1920:C:N4     | 2.36        | 0.58     |
| 1:A:259:G:H21    | 1:A:621:A:H8      | 1.51        | 0.58     |
| 3:C:71:ASP:OD2   | 3:C:103:ARG:NH2   | 2.36        | 0.58     |
| 6:F:112:PRO:HB3  | 26:Z:37:SER:HB2   | 1.85        | 0.58     |
| 21:U:158:PRO:HG2 | 21:U:161:VAL:HG21 | 1.85        | 0.58     |
| 1:A:102:G:H4'    | 1:A:103:A:O5'     | 2.03        | 0.58     |
| 3:C:44:ASN:CB    | 3:C:49:ILE:HA     | 2.33        | 0.58     |
| 8:H:55:ALA:HA    | 8:H:58:LEU:CB     | 2.32        | 0.58     |
| 4:D:13:ARG:HH11  | 4:D:21:VAL:HG11   | 1.68        | 0.58     |
| 8:H:110:ASP:N    | 8:H:130:TYR:OH    | 2.30        | 0.58     |
| 21:U:110:GLY:HA2 | 21:U:112:ARG:HB2  | 1.84        | 0.58     |
| 1:A:1226:G:H4'   | 17:Q:84:LYS:HG2   | 1.84        | 0.58     |
| 1:A:1579:A:H2'   | 1:A:1580:A:C8     | 2.38        | 0.58     |
| 1:A:1899:G:H21   | 1:A:1902:C:N4     | 2.01        | 0.58     |
| 3:C:182:LEU:N    | 3:C:272:ALA:HB3   | 2.17        | 0.58     |
| 1:A:2680:C:H5'   | 4:D:189:PRO:HA    | 1.84        | 0.58     |
| 6:F:136:ARG:O    | 6:F:154:GLY:HA2   | 2.03        | 0.58     |
| 7:G:89:ILE:O     | 7:G:89:ILE:HG12   | 2.04        | 0.58     |
| 1:A:2126:A:H4'   | 1:A:2127:G:O5'    | 2.04        | 0.58     |
| 3:C:35:LYS:HD2   | 3:C:104:TYR:CE1   | 2.39        | 0.58     |
| 7:G:87:LEU:HD22  | 7:G:162:ILE:HG22  | 1.85        | 0.58     |
| 12:L:78:PRO:O    | 22:V:5:LYS:HE2    | 2.03        | 0.58     |
| 1:A:654(A):G:H1  | 1:A:654(T):C:H42  | 1.49        | 0.58     |
| 3:C:24:ILE:HD11  | 3:C:91:ARG:HD2    | 1.84        | 0.58     |
| 8:H:5:LEU:HD12   | 8:H:5:LEU:H       | 1.69        | 0.58     |
| 1:A:1266:G:O5'   | 18:R:15:ARG:NH2   | 2.37        | 0.58     |
| 11:K:47:ASP:OD2  | 11:K:49:ARG:NH1   | 2.37        | 0.58     |
| 9:I:54:VAL:HB    | 9:I:122:VAL:HG22  | 1.85        | 0.58     |
| 1:A:414:C:O2     | 1:A:1864:U:O2'    | 2.21        | 0.57     |
| 1:A:65:C:O2'     | 1:A:456:C:N3      | 2.33        | 0.57     |
| 2:B:44:G:OP1     | 26:Z:1:MET:N      | 2.35        | 0.57     |
| 4:D:131:ALA:HB1  | 4:D:135:HIS:HE1   | 1.69        | 0.57     |
| 9:I:13:TRP:O     | 9:I:135:PRO:HD2   | 2.03        | 0.57     |
| 12:L:135:ASP:OD2 | 21:U:81:ARG:NH1   | 2.37        | 0.57     |
| 20:T:95:LYS:NZ   | 20:T:99:CYS:O     | 2.37        | 0.57     |
| 6:F:68:PRO:HB2   | 6:F:90:LEU:HD12   | 1.86        | 0.57     |
| 18:R:71:VAL:HA   | 18:R:107:LEU:HD12 | 1.86        | 0.57     |
| 1:A:1490:A:O2'   | 3:C:99:ASP:OD1    | 2.21        | 0.57     |
| 7:G:153:LYS:HB3  | 7:G:154:PRO:CD    | 2.34        | 0.57     |
| 12:L:81:VAL:HG23 | 22:V:7:LEU:CD1    | 2.34        | 0.57     |
| 22:V:18:ALA:O    | 22:V:20:ARG:NH1   | 2.36        | 0.57     |

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| Atom-1           | Atom-2            | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:A:330:A:H2     | 1:A:1210:A:H2'    | 1.70        | 0.57     |
| 1:A:307:G:N2     | 1:A:309:G:H3'     | 2.20        | 0.57     |
| 3:C:145:VAL:HG13 | 3:C:191:ALA:HB2   | 1.87        | 0.57     |
| 13:M:117:VAL:O   | 13:M:118:GLU:HB2  | 2.05        | 0.57     |
| 20:T:76:CYS:SG   | 20:T:77:PRO:HD2   | 2.45        | 0.57     |
| 1:A:137(A):G:H1' | 19:S:41:ASN:ND2   | 2.19        | 0.57     |
| 1:A:1045:A:C4    | 1:A:1111:A:N6     | 2.73        | 0.57     |
| 1:A:1341:U:OP2   | 1:A:1394:U:O2'    | 2.19        | 0.57     |
| 1:A:1936:A:OP2   | 1:A:1962:C:N4     | 2.37        | 0.57     |
| 1:A:2735:G:H2'   | 1:A:2736:G:H8     | 1.67        | 0.57     |
| 3:C:241:PRO:O    | 3:C:242:ARG:HB2   | 2.04        | 0.57     |
| 6:F:22:ARG:HH21  | 6:F:171:ALA:HB1   | 1.69        | 0.57     |
| 11:K:58:THR:C    | 11:K:61:ARG:HE    | 2.06        | 0.57     |
| 1:A:247:G:H4'    | 1:A:386:G:C5      | 2.40        | 0.57     |
| 3:C:44:ASN:HB2   | 3:C:48:ARG:O      | 2.05        | 0.57     |
| 15:O:41:ARG:CZ   | 15:O:41:ARG:HB2   | 2.34        | 0.57     |
| 1:A:2335:A:O2'   | 1:A:2336:A:O5'    | 2.23        | 0.56     |
| 17:Q:52:VAL:HG21 | 17:Q:55:ALA:HB3   | 1.87        | 0.56     |
| 1:A:1454:U:OP1   | 13:M:77:ARG:NH1   | 2.34        | 0.56     |
| 3:C:108:PRO:HB3  | 3:C:143:HIS:CE1   | 2.40        | 0.56     |
| 3:C:148:GLU:HB2  | 3:C:151:LYS:HD2   | 1.87        | 0.56     |
| 20:T:81:LYS:HZ3  | 20:T:98:VAL:HG11  | 1.69        | 0.56     |
| 1:A:1316:U:H2'   | 1:A:1317:A:C8     | 2.41        | 0.56     |
| 4:D:13:ARG:CB    | 4:D:21:VAL:CG1    | 2.83        | 0.56     |
| 5:E:11:VAL:HG12  | 5:E:12:LEU:H      | 1.69        | 0.56     |
| 8:H:116:LEU:O    | 8:H:118:LYS:N     | 2.38        | 0.56     |
| 11:K:106:LEU:O   | 11:K:107:LYS:HB2  | 2.05        | 0.56     |
| 12:L:24:GLY:O    | 12:L:26:TYR:N     | 2.36        | 0.56     |
| 12:L:32:TYR:HE1  | 12:L:133:ARG:HG3  | 1.69        | 0.56     |
| 4:D:15:PHE:CD1   | 4:D:20:ALA:CB     | 2.87        | 0.56     |
| 1:A:443:A:C5     | 5:E:45:ARG:HD2    | 2.41        | 0.56     |
| 1:A:443:A:N7     | 5:E:45:ARG:HD2    | 2.20        | 0.56     |
| 8:H:52:ARG:C     | 8:H:56:LYS:H      | 2.03        | 0.56     |
| 12:L:43:THR:HA   | 12:L:94:VAL:HG12  | 1.88        | 0.56     |
| 14:N:106:ARG:HA  | 14:N:110:LEU:HD11 | 1.87        | 0.56     |
| 1:A:1337:G:OP2   | 19:S:73:ARG:NH2   | 2.38        | 0.56     |
| 1:A:2212:A:H1'   | 1:A:2215:G:C5     | 2.40        | 0.56     |
| 4:D:10:GLY:HA3   | 15:O:8:LYS:HD2    | 1.85        | 0.56     |
| 12:L:66:ILE:HA   | 12:L:104:PHE:HA   | 1.87        | 0.56     |
| 13:M:67:LEU:HD13 | 13:M:76:VAL:HG21  | 1.86        | 0.56     |
| 17:Q:44:LYS:HE2  | 17:Q:45:THR:H     | 1.70        | 0.56     |
| 1:A:1012:U:O2'   | 1:A:1013:C:OP2    | 2.19        | 0.56     |

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| Atom-1            | Atom-2           | Distance(Å) | Clash(Å) |
|-------------------|------------------|-------------|----------|
| 4:D:4:ILE:HD12    | 4:D:28:ALA:HB1   | 1.88        | 0.56     |
| 21:U:111:VAL:HG13 | 21:U:112:ARG:N   | 2.19        | 0.56     |
| 8:H:8:PRO:HD3     | 8:H:15:VAL:HG13  | 1.87        | 0.56     |
| 1:A:27:G:O2'      | 1:A:28:A:O5'     | 2.23        | 0.56     |
| 8:H:29:TYR:HD2    | 8:H:30:LEU:HD23  | 1.71        | 0.56     |
| 1:A:2690:C:OP2    | 13:M:14:SER:HB3  | 2.06        | 0.56     |
| 1:A:1509:C:H3'    | 1:A:1510:A:H5''  | 1.88        | 0.56     |
| 1:A:1754:C:OP1    | 15:O:96:ARG:NH1  | 2.34        | 0.56     |
| 1:A:793:A:OP2     | 1:A:2071:A:O2'   | 2.22        | 0.56     |
| 8:H:41:GLU:HA     | 8:H:44:LEU:HB2   | 1.87        | 0.56     |
| 19:S:31:HIS:CD2   | 19:S:32:PRO:HD2  | 2.41        | 0.56     |
| 21:U:182:LYS:H    | 21:U:182:LYS:HD3 | 1.70        | 0.56     |
| 5:E:24:LEU:CD2    | 5:E:115:ALA:HA   | 2.36        | 0.55     |
| 11:K:121:LYS:HD3  | 11:K:122:PRO:HD2 | 1.88        | 0.55     |
| 15:O:26:ASP:O     | 15:O:49:VAL:HG12 | 2.07        | 0.55     |
| 1:A:2404:C:H1'    | 11:K:67:MET:HE1  | 1.88        | 0.55     |
| 5:E:110:LEU:HD11  | 5:E:181:LEU:HD12 | 1.88        | 0.55     |
| 8:H:92:VAL:HG13   | 8:H:120:ILE:HG23 | 1.88        | 0.55     |
| 26:Z:24:THR:OG1   | 26:Z:25:TYR:N    | 2.38        | 0.55     |
| 1:A:1417:C:H2'    | 1:A:1418:G:O4'   | 2.05        | 0.55     |
| 4:D:63:LEU:CD1    | 4:D:65:GLY:H     | 2.20        | 0.55     |
| 23:W:53:VAL:HG11  | 23:W:90:ILE:HD11 | 1.88        | 0.55     |
| 8:H:21:VAL:HG21   | 8:H:25:TYR:HD2   | 1.71        | 0.55     |
| 8:H:52:ARG:O      | 8:H:56:LYS:CA    | 2.55        | 0.55     |
| 10:J:78:ARG:HH21  | 15:O:103:ARG:NH2 | 2.03        | 0.55     |
| 17:Q:7:THR:HG23   | 17:Q:22:VAL:HG11 | 1.88        | 0.55     |
| 18:R:86:LEU:HD22  | 18:R:96:ILE:HD11 | 1.88        | 0.55     |
| 1:A:181:A:H1'     | 1:A:435:C:H5'    | 1.88        | 0.55     |
| 5:E:101:LEU:O     | 5:E:106:ARG:NH1  | 2.40        | 0.55     |
| 8:H:94:ALA:H      | 8:H:116:LEU:HD13 | 1.71        | 0.55     |
| 20:T:81:LYS:HB2   | 20:T:96:ILE:HG22 | 1.89        | 0.55     |
| 20:T:95:LYS:CB    | 20:T:100:ALA:HA  | 2.36        | 0.55     |
| 1:A:1045:A:N9     | 1:A:1111:A:N6    | 2.55        | 0.55     |
| 1:A:1141:U:H1'    | 1:A:1142(A):A:C6 | 2.42        | 0.55     |
| 3:C:35:LYS:NZ     | 3:C:104:TYR:HB2  | 2.21        | 0.55     |
| 1:A:535:C:O3'     | 16:P:53:ARG:NH1  | 2.39        | 0.55     |
| 20:T:96:ILE:HG12  | 20:T:101:LYS:HB2 | 1.88        | 0.55     |
| 26:Z:16:CYS:SG    | 26:Z:36:CYS:N    | 2.79        | 0.55     |
| 1:A:1316:U:H2'    | 1:A:1317:A:H8    | 1.71        | 0.55     |
| 1:A:2805:G:H2'    | 1:A:2807:G:C8    | 2.41        | 0.55     |
| 16:P:52:ARG:HA    | 16:P:55:ARG:HG3  | 1.87        | 0.55     |
| 20:T:37:VAL:HG21  | 20:T:72:VAL:HG21 | 1.88        | 0.55     |

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| Atom-1           | Atom-2            | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:A:807:U:H2'    | 1:A:808:G:C8      | 2.41        | 0.55     |
| 12:L:30:GLY:CA   | 12:L:107:ALA:HB2  | 2.37        | 0.55     |
| 7:G:109:PHE:HZ   | 7:G:152:ARG:HG2   | 1.72        | 0.55     |
| 1:A:1689:A:H2'   | 1:A:1690:A:H8     | 1.72        | 0.55     |
| 5:E:24:LEU:HG    | 5:E:115:ALA:CB    | 2.37        | 0.55     |
| 7:G:124:GLU:HB3  | 7:G:132:ARG:HG3   | 1.89        | 0.55     |
| 15:O:1:MET:O     | 15:O:3:ARG:N      | 2.40        | 0.55     |
| 1:A:1021:A:N6    | 1:A:1142(A):A:H61 | 2.02        | 0.54     |
| 1:A:1359:A:N6    | 1:A:1372:U:C4     | 2.75        | 0.54     |
| 1:A:2335:A:O2'   | 1:A:2336:A:H2'    | 2.07        | 0.54     |
| 5:E:184:TYR:CE2  | 5:E:188:ARG:HD2   | 2.42        | 0.54     |
| 12:L:31:ASP:O    | 12:L:134:ARG:HB2  | 2.07        | 0.54     |
| 24:X:42:GLY:O    | 24:X:44:LEU:N     | 2.35        | 0.54     |
| 1:A:1085:A:O2'   | 1:A:1086:A:OP1    | 2.24        | 0.54     |
| 1:A:622:G:OP2    | 11:K:108:LYS:NZ   | 2.29        | 0.54     |
| 2:B:38:C:N3      | 2:B:44:G:N2       | 2.42        | 0.54     |
| 9:I:30:ILE:HG22  | 9:I:34:LEU:HD22   | 1.88        | 0.54     |
| 19:S:25:LYS:HD3  | 19:S:80:ILE:HD11  | 1.89        | 0.54     |
| 1:A:686:G:H21    | 1:A:788:A:H61     | 1.54        | 0.54     |
| 9:I:40:PRO:HB3   | 16:P:68:ALA:HB2   | 1.89        | 0.54     |
| 12:L:54:MET:HG3  | 12:L:117:ALA:HB1  | 1.89        | 0.54     |
| 1:A:307:G:H21    | 1:A:330:A:H62     | 1.55        | 0.54     |
| 3:C:35:LYS:HZ1   | 3:C:104:TYR:HB2   | 1.71        | 0.54     |
| 4:D:35:GLN:HE21  | 4:D:37:ARG:CZ     | 2.21        | 0.54     |
| 1:A:442:G:H1'    | 5:E:48:THR:HG21   | 1.89        | 0.54     |
| 8:H:113:ARG:HG3  | 8:H:131:LYS:NZ    | 2.23        | 0.54     |
| 21:U:146:ILE:HA  | 21:U:174:VAL:HB   | 1.90        | 0.54     |
| 6:F:16:ARG:NH2   | 6:F:28:VAL:O      | 2.41        | 0.54     |
| 8:H:93:THR:O     | 8:H:97:ILE:HG12   | 2.06        | 0.54     |
| 1:A:642:G:H21    | 1:A:646:A:H2      | 1.55        | 0.54     |
| 13:M:103:ARG:NH1 | 13:M:108:GLY:O    | 2.41        | 0.54     |
| 1:A:2292:C:OP1   | 14:N:17:ARG:NH2   | 2.40        | 0.54     |
| 16:P:112:ARG:NH2 | 17:Q:47:VAL:HG13  | 2.23        | 0.54     |
| 19:S:83:VAL:CG1  | 19:S:87:GLN:HB2   | 2.38        | 0.54     |
| 21:U:53:ILE:H    | 21:U:71:VAL:HG13  | 1.72        | 0.54     |
| 23:W:58:ILE:HD11 | 23:W:86:SER:HB2   | 1.88        | 0.54     |
| 24:X:50:ILE:HD12 | 24:X:51:ARG:H     | 1.73        | 0.54     |
| 1:A:1453:A:N6    | 1:A:2702:U:H1'    | 2.23        | 0.54     |
| 1:A:2068:U:N3    | 1:A:2430:A:H2     | 2.04        | 0.54     |
| 1:A:78:A:H2'     | 1:A:79:G:H8       | 1.73        | 0.54     |
| 2:B:44:G:H1'     | 2:B:47:C:H42      | 1.71        | 0.54     |
| 2:B:52:A:N6      | 14:N:33:LYS:HG3   | 2.23        | 0.54     |

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| Atom-1           | Atom-2            | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 11:K:38:GLN:HG2  | 11:K:45:LEU:CD1   | 2.36        | 0.54     |
| 15:O:111:ARG:O   | 15:O:112:ARG:HG3  | 2.08        | 0.54     |
| 1:A:1359:A:C6    | 1:A:1372:U:C4     | 2.96        | 0.54     |
| 11:K:14:LYS:O    | 11:K:16:ARG:HG2   | 2.08        | 0.54     |
| 1:A:2469:A:H5''  | 1:A:2470:G:C8     | 2.43        | 0.54     |
| 1:A:2543:G:H21   | 1:A:2646:C:H5''   | 1.73        | 0.54     |
| 21:U:82:ARG:HG3  | 21:U:83:PRO:HD2   | 1.90        | 0.54     |
| 1:A:1268:A:H2'   | 1:A:1269:A:O4'    | 2.07        | 0.54     |
| 1:A:2441:C:OP2   | 1:A:2586:C:O2'    | 2.25        | 0.54     |
| 1:A:2725:A:O2'   | 1:A:2726:U:H5''   | 2.08        | 0.54     |
| 1:A:288:C:H2'    | 1:A:289:A:C8      | 2.42        | 0.54     |
| 1:A:574:C:N3     | 4:D:145:LYS:NZ    | 2.55        | 0.54     |
| 1:A:947:G:H2'    | 1:A:948:G:C8      | 2.42        | 0.54     |
| 4:D:111:ARG:HG3  | 4:D:160:TYR:CD2   | 2.43        | 0.54     |
| 1:A:2786:U:O2'   | 4:D:62:PRO:O      | 2.23        | 0.54     |
| 8:H:33:ARG:HB3   | 8:H:35:LEU:HD23   | 1.90        | 0.54     |
| 13:M:45:ARG:HA   | 13:M:95:THR:HG21  | 1.90        | 0.54     |
| 15:O:37:GLY:O    | 15:O:39:ARG:N     | 2.34        | 0.54     |
| 1:A:551:G:H5'    | 1:A:1220:A:H1'    | 1.89        | 0.53     |
| 3:C:44:ASN:HD22  | 3:C:44:ASN:N      | 2.06        | 0.53     |
| 1:A:1754:C:H5''  | 15:O:113:LYS:HE3  | 1.90        | 0.53     |
| 21:U:76:LEU:H    | 21:U:76:LEU:HD23  | 1.73        | 0.53     |
| 26:Z:56:VAL:HA   | 26:Z:60:GLN:HB2   | 1.89        | 0.53     |
| 1:A:2126:A:N6    | 1:A:2163:C:O2'    | 2.42        | 0.53     |
| 1:A:519:U:H2'    | 1:A:520:G:H8      | 1.73        | 0.53     |
| 1:A:882:G:H1     | 1:A:894:C:N4      | 2.02        | 0.53     |
| 1:A:974(A):C:H4' | 1:A:975:G:O5'     | 2.08        | 0.53     |
| 4:D:21:VAL:CG2   | 4:D:22:PRO:CB     | 2.58        | 0.53     |
| 21:U:152:ALA:O   | 21:U:154:ASP:N    | 2.40        | 0.53     |
| 1:A:1149:G:H2'   | 1:A:1150:C:C6     | 2.43        | 0.53     |
| 1:A:2844:G:H3'   | 1:A:2845:G:H8     | 1.74        | 0.53     |
| 4:D:13:ARG:HD2   | 11:K:61:ARG:HD2   | 122.65      | 0.53     |
| 5:E:32:LEU:O     | 5:E:36:VAL:HG23   | 2.09        | 0.53     |
| 7:G:149:ARG:HE   | 7:G:154:PRO:HG2   | 1.72        | 0.53     |
| 14:N:106:ARG:HA  | 14:N:110:LEU:HD21 | 1.90        | 0.53     |
| 15:O:33:LYS:HD2  | 15:O:82:LEU:HA    | 1.89        | 0.53     |
| 21:U:58:VAL:O    | 21:U:60:GLU:N     | 2.39        | 0.53     |
| 1:A:1419:A:H61   | 1:A:1494:A:H61    | 1.55        | 0.53     |
| 1:A:1411:C:N4    | 1:A:1591:G:H1     | 2.04        | 0.53     |
| 12:L:32:TYR:CE1  | 12:L:133:ARG:HG3  | 2.43        | 0.53     |
| 17:Q:99:ILE:O    | 17:Q:101:GLY:N    | 2.41        | 0.53     |
| 21:U:166:SER:H   | 21:U:167:PRO:HA   | 1.74        | 0.53     |

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| Atom-1           | Atom-2            | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:A:49:A:C8      | 1:A:120:U:C5      | 2.97        | 0.53     |
| 10:J:2:ILE:HD13  | 10:J:8:LEU:HD11   | 1.90        | 0.53     |
| 21:U:5:LEU:HD11  | 21:U:39:VAL:HB    | 1.91        | 0.53     |
| 24:X:65:ASN:HB3  | 24:X:69:ARG:NH2   | 2.24        | 0.53     |
| 1:A:1799:G:H4'   | 1:A:1800:C:O5'    | 2.08        | 0.53     |
| 1:A:1798:U:C5'   | 3:C:259:THR:HG22  | 2.38        | 0.53     |
| 1:A:1861:G:H1    | 1:A:1881:C:H42    | 1.54        | 0.53     |
| 4:D:203:LYS:HE3  | 4:D:204:ALA:HB2   | 1.90        | 0.53     |
| 5:E:135:LYS:HB3  | 5:E:138:GLU:HG3   | 1.90        | 0.53     |
| 8:H:88:ILE:O     | 8:H:121:LYS:NZ    | 2.40        | 0.53     |
| 11:K:113:LYS:HG2 | 11:K:115:LEU:HD23 | 1.90        | 0.53     |
| 20:T:98:VAL:HG13 | 20:T:99:CYS:SG    | 2.48        | 0.53     |
| 24:X:10:LEU:O    | 24:X:13:ALA:N     | 2.40        | 0.53     |
| 1:A:1050:A:H2'   | 1:A:1051:G:O4'    | 2.09        | 0.53     |
| 1:A:1358:G:N1    | 1:A:1372:U:OP2    | 2.25        | 0.53     |
| 3:C:206:LEU:O    | 3:C:211:ARG:NH1   | 2.38        | 0.53     |
| 4:D:1:MET:N      | 4:D:83:ASP:O      | 2.41        | 0.53     |
| 5:E:157:VAL:HB   | 5:E:194:MET:HB3   | 1.91        | 0.53     |
| 1:A:1165:U:H2'   | 1:A:1166:C:C6     | 2.44        | 0.53     |
| 1:A:2482:G:O6    | 12:L:124:LYS:NZ   | 2.42        | 0.53     |
| 4:D:21:VAL:CB    | 4:D:22:PRO:CA     | 2.87        | 0.53     |
| 18:R:110:LYS:HG3 | 18:R:111:HIS:ND1  | 2.23        | 0.53     |
| 23:W:80:LEU:HD23 | 23:W:80:LEU:H     | 1.74        | 0.53     |
| 7:G:10:PRO:HD2   | 7:G:50:VAL:HG13   | 1.89        | 0.52     |
| 8:H:144:VAL:HG22 | 8:H:145:VAL:H     | 1.73        | 0.52     |
| 1:A:2503:A:O2'   | 1:A:2505:G:OP2    | 2.24        | 0.52     |
| 1:A:347:A:H2'    | 1:A:348:G:H8      | 1.73        | 0.52     |
| 5:E:134:GLY:HA3  | 5:E:165:ARG:NH1   | 2.25        | 0.52     |
| 7:G:46:GLU:OE2   | 7:G:51:ARG:NH1    | 2.42        | 0.52     |
| 3:C:133:LEU:HB3  | 3:C:173:VAL:HG11  | 1.91        | 0.52     |
| 1:A:443:A:H3'    | 5:E:45:ARG:NH1    | 2.23        | 0.52     |
| 6:F:82:LEU:HA    | 6:F:86:MET:SD     | 2.48        | 0.52     |
| 2:B:52:A:H62     | 14:N:33:LYS:HG3   | 1.73        | 0.52     |
| 17:Q:60:GLU:HB2  | 17:Q:97:LYS:HE3   | 1.91        | 0.52     |
| 1:A:2308:G:O6    | 1:A:2311:A:N1     | 2.42        | 0.52     |
| 3:C:35:LYS:NZ    | 3:C:64:ILE:O      | 2.41        | 0.52     |
| 7:G:86:GLU:HG3   | 7:G:165:ALA:N     | 2.25        | 0.52     |
| 8:H:11:ASN:O     | 8:H:12:LEU:HB2    | 2.09        | 0.52     |
| 1:A:1357:U:H2'   | 1:A:1358:G:O4'    | 2.09        | 0.52     |
| 1:A:1869:G:H5'   | 1:A:1870:C:OP2    | 2.09        | 0.52     |
| 1:A:2438:U:O3'   | 1:A:2439:A:H3'    | 2.09        | 0.52     |
| 1:A:637:A:O5'    | 11:K:116:GLY:HA2  | 2.08        | 0.52     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 8:H:55:ALA:C     | 8:H:58:LEU:HB3   | 2.30        | 0.52     |
| 13:M:59:ASP:OD2  | 13:M:61:HIS:HB3  | 2.08        | 0.52     |
| 12:L:81:VAL:HG23 | 22:V:7:LEU:HD11  | 1.91        | 0.52     |
| 1:A:1311:G:H21   | 1:A:1603:A:N6    | 2.06        | 0.52     |
| 1:A:2693:A:H2'   | 1:A:2694:G:C8    | 2.44        | 0.52     |
| 1:A:345:A:H2'    | 1:A:347:A:H62    | 1.74        | 0.52     |
| 3:C:108:PRO:HB3  | 3:C:143:HIS:HE1  | 1.73        | 0.52     |
| 24:X:4:SER:OG    | 24:X:5:GLU:OE2   | 2.16        | 0.52     |
| 1:A:1980:G:H4'   | 1:A:1981:A:OP2   | 2.09        | 0.52     |
| 1:A:631:A:OP1    | 11:K:64:LYS:HE2  | 2.10        | 0.52     |
| 3:C:206:LEU:HD22 | 3:C:211:ARG:HG2  | 1.92        | 0.52     |
| 1:A:608:A:OP1    | 5:E:100:THR:OG1  | 2.27        | 0.52     |
| 1:A:2232:U:P     | 23:W:40:ARG:HH12 | 2.33        | 0.52     |
| 1:A:2146:C:H4'   | 1:A:2147:G:C8    | 2.44        | 0.52     |
| 1:A:38:A:H2'     | 1:A:39:C:C6      | 2.45        | 0.52     |
| 5:E:150:GLY:HA2  | 5:E:172:TRP:CE3  | 2.44        | 0.52     |
| 1:A:1244:G:H4'   | 11:K:7:ARG:HB2   | 1.92        | 0.52     |
| 1:A:1264:G:H3'   | 1:A:1265:A:H5''  | 1.90        | 0.52     |
| 1:A:1689:A:H2'   | 1:A:1690:A:C8    | 2.44        | 0.52     |
| 1:A:2776:A:H4'   | 1:A:2777:G:O5'   | 2.09        | 0.52     |
| 8:H:133:HIS:HB2  | 8:H:134:PRO:HD2  | 1.92        | 0.52     |
| 1:A:1007:C:H5''  | 9:I:35:ARG:NH1   | 2.25        | 0.52     |
| 13:M:33:ARG:HD3  | 13:M:113:LEU:HG  | 1.92        | 0.52     |
| 1:A:25:U:H5'     | 18:R:79:GLY:HA2  | 1.91        | 0.52     |
| 20:T:84:ARG:O    | 20:T:95:LYS:HD3  | 2.09        | 0.52     |
| 21:U:111:VAL:CG2 | 21:U:112:ARG:H   | 2.12        | 0.52     |
| 23:W:2:SER:HB2   | 23:W:4:VAL:HG12  | 1.92        | 0.52     |
| 1:A:818:G:N1     | 1:A:1188:U:OP2   | 2.28        | 0.52     |
| 18:R:60:ASN:HD22 | 18:R:60:ASN:H    | 1.56        | 0.52     |
| 20:T:87:LYS:HA   | 20:T:92:ASN:HB3  | 1.91        | 0.52     |
| 21:U:5:LEU:HD21  | 21:U:44:PHE:HA   | 1.92        | 0.52     |
| 1:A:1543:A:C1'   | 1:A:1545:A:O4'   | 2.53        | 0.51     |
| 1:A:177:G:H3'    | 1:A:178:G:H8     | 1.74        | 0.51     |
| 1:A:1942:C:OP2   | 1:A:1943:U:O2'   | 2.24        | 0.51     |
| 1:A:2123:G:H2'   | 1:A:2124:G:H8    | 1.74        | 0.51     |
| 2:B:111:U:H2'    | 2:B:112:G:H8     | 1.75        | 0.51     |
| 17:Q:34:GLU:O    | 17:Q:36:PRO:HD3  | 2.10        | 0.51     |
| 1:A:1598:C:H5'   | 19:S:36:LYS:HB2  | 1.91        | 0.51     |
| 2:B:74:U:H1'     | 21:U:34:ASN:HD21 | 1.74        | 0.51     |
| 1:A:1899:G:H21   | 1:A:1902:C:H41   | 1.57        | 0.51     |
| 3:C:12:SER:HB2   | 3:C:208:LYS:HB3  | 1.92        | 0.51     |
| 5:E:150:GLY:HA2  | 5:E:172:TRP:CD2  | 2.45        | 0.51     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 5:E:47:GLY:HA3   | 5:E:95:ARG:O     | 2.10        | 0.51     |
| 7:G:86:GLU:CD    | 7:G:86:GLU:H     | 2.12        | 0.51     |
| 1:A:2126:A:H2    | 1:A:2162:G:H21   | 1.59        | 0.51     |
| 7:G:153:LYS:HG2  | 7:G:162:ILE:HG13 | 1.92        | 0.51     |
| 15:O:111:ARG:C   | 15:O:113:LYS:H   | 2.12        | 0.51     |
| 19:S:35:THR:HG23 | 19:S:38:GLU:HG2  | 1.92        | 0.51     |
| 20:T:74:PRO:O    | 20:T:80:GLY:HA2  | 2.10        | 0.51     |
| 1:A:347:A:H2'    | 1:A:348:G:C8     | 2.45        | 0.51     |
| 1:A:806:C:P      | 11:K:41:ARG:HH11 | 2.31        | 0.51     |
| 2:B:50:G:H5''    | 14:N:61:ASN:ND2  | 2.26        | 0.51     |
| 16:P:90:VAL:HG22 | 17:Q:39:LEU:HB3  | 1.93        | 0.51     |
| 1:A:391:G:O2'    | 1:A:410:G:OP1    | 2.26        | 0.51     |
| 4:D:23:VAL:HA    | 4:D:184:VAL:O    | 2.11        | 0.51     |
| 19:S:59:VAL:HG21 | 19:S:78:LYS:HE3  | 1.91        | 0.51     |
| 1:A:2121:G:O6    | 1:A:2176:A:N6    | 2.43        | 0.51     |
| 2:B:15:A:H5'     | 2:B:16:G:C8      | 2.45        | 0.51     |
| 4:D:134:ILE:HA   | 4:D:137:HIS:CD2  | 2.45        | 0.51     |
| 5:E:185:ASP:HA   | 5:E:188:ARG:HD3  | 1.93        | 0.51     |
| 8:H:52:ARG:CB    | 8:H:56:LYS:HB2   | 2.32        | 0.51     |
| 1:A:1403:C:H5''  | 1:A:1471:A:H1'   | 1.92        | 0.51     |
| 1:A:1543:A:H2    | 1:A:1545:A:C5    | 2.29        | 0.51     |
| 1:A:67:U:H3      | 1:A:74:A:H2      | 1.54        | 0.51     |
| 2:B:16:G:H1      | 2:B:68:C:H42     | 1.59        | 0.51     |
| 5:E:20:LEU:HD23  | 5:E:125:LEU:HD12 | 1.93        | 0.51     |
| 6:F:88:ILE:O     | 6:F:88:ILE:HD13  | 2.10        | 0.51     |
| 7:G:127:GLU:CB   | 7:G:130:ARG:HB3  | 2.40        | 0.51     |
| 14:N:56:LEU:HD23 | 14:N:58:LEU:HD22 | 1.92        | 0.51     |
| 15:O:28:VAL:HG23 | 15:O:88:ILE:HA   | 1.92        | 0.51     |
| 8:H:55:ALA:HA    | 8:H:58:LEU:HB3   | 1.93        | 0.51     |
| 18:R:67:ASP:OD1  | 18:R:67:ASP:N    | 2.33        | 0.51     |
| 19:S:40:LYS:HG3  | 19:S:51:VAL:HB   | 1.92        | 0.51     |
| 1:A:1009:A:OP2   | 1:A:1010:A:OP2   | 2.28        | 0.51     |
| 1:A:1203:G:O6    | 1:A:1204:A:N6    | 2.44        | 0.51     |
| 1:A:693:C:O2'    | 1:A:1353:A:N3    | 2.41        | 0.51     |
| 1:A:2443:C:H2'   | 1:A:2444:G:C8    | 2.44        | 0.51     |
| 1:A:2832:U:H4'   | 1:A:2833:G:H5''  | 1.92        | 0.51     |
| 12:L:20:ALA:HB3  | 21:U:79:ARG:NH1  | 2.26        | 0.51     |
| 1:A:111:A:H4'    | 24:X:69:ARG:NH2  | 2.26        | 0.50     |
| 1:A:1443:G:H1    | 1:A:1548:C:N4    | 2.04        | 0.50     |
| 1:A:458:G:O2'    | 1:A:469:G:O6     | 2.19        | 0.50     |
| 4:D:176:ILE:HG23 | 4:D:178:GLU:OE2  | 2.11        | 0.50     |
| 11:K:14:LYS:O    | 11:K:14:LYS:HD3  | 2.11        | 0.50     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 15:O:118:ARG:HH21 | 15:O:121:ILE:HG21 | 1.76        | 0.50     |
| 15:O:19:LEU:HD22  | 15:O:86:ILE:HG22  | 1.93        | 0.50     |
| 20:T:97:ARG:HH21  | 20:T:98:VAL:HB    | 1.77        | 0.50     |
| 1:A:1363:C:O2'    | 1:A:1809:A:N3     | 2.37        | 0.50     |
| 9:I:46:VAL:HG13   | 9:I:48:MET:HG3    | 1.93        | 0.50     |
| 12:L:17:LEU:HD23  | 12:L:96:VAL:HG23  | 1.92        | 0.50     |
| 1:A:94:G:H21      | 24:X:47:ASN:HD22  | 1.59        | 0.50     |
| 1:A:1427:A:H4'    | 1:A:1428:C:O5'    | 2.10        | 0.50     |
| 1:A:2777:G:OP2    | 1:A:2781:A:O2'    | 2.23        | 0.50     |
| 1:A:620:G:H4'     | 1:A:621:A:H5''    | 1.94        | 0.50     |
| 7:G:132:ARG:HB2   | 7:G:132:ARG:HH11  | 1.76        | 0.50     |
| 4:D:6:GLY:HA2     | 4:D:51:PHE:CZ     | 2.46        | 0.50     |
| 12:L:89:ASN:O     | 12:L:92:GLY:N     | 2.42        | 0.50     |
| 1:A:2789:C:H1'    | 1:A:2892:A:H2     | 1.75        | 0.50     |
| 1:A:1205:U:C4     | 5:E:171:PRO:HA    | 2.46        | 0.50     |
| 15:O:111:ARG:O    | 15:O:113:LYS:N    | 2.42        | 0.50     |
| 18:R:60:ASN:N     | 18:R:60:ASN:HD22  | 2.09        | 0.50     |
| 1:A:407:G:H2'     | 1:A:408:G:C8      | 2.46        | 0.50     |
| 1:A:1140:C:OP1    | 9:I:23:LEU:HB3    | 2.10        | 0.50     |
| 15:O:39:ARG:HG2   | 15:O:40:THR:H     | 1.76        | 0.50     |
| 21:U:91:LEU:HD11  | 21:U:96:VAL:HG21  | 1.92        | 0.50     |
| 23:W:62:VAL:HG23  | 23:W:63:ALA:O     | 2.11        | 0.50     |
| 1:A:1542:G:C3'    | 1:A:1543:A:C5'    | 2.76        | 0.50     |
| 1:A:2306:C:H2'    | 1:A:2307:G:N2     | 2.26        | 0.50     |
| 1:A:259:G:O2'     | 1:A:621:A:O2'     | 2.24        | 0.50     |
| 1:A:760:G:H2'     | 1:A:761:A:O4'     | 2.12        | 0.50     |
| 5:E:16:GLY:O      | 5:E:18:ARG:N      | 2.45        | 0.50     |
| 8:H:29:TYR:O      | 8:H:33:ARG:HB2    | 2.12        | 0.50     |
| 1:A:270(L):U:H2'  | 8:H:50:ARG:HD2    | 1.94        | 0.50     |
| 11:K:26:GLY:O     | 11:K:28:GLY:N     | 2.45        | 0.50     |
| 1:A:2277:G:OP2    | 22:V:10:THR:HG21  | 2.11        | 0.50     |
| 1:A:1790:C:H5''   | 1:A:1791:A:OP1    | 2.11        | 0.50     |
| 1:A:2103:C:H42    | 1:A:2186:G:H1     | 1.59        | 0.50     |
| 1:A:270(H):C:H42  | 1:A:270(R):G:H1   | 1.60        | 0.50     |
| 3:C:62:TYR:CE2    | 3:C:64:ILE:HA     | 2.46        | 0.50     |
| 12:L:134:ARG:NH2  | 21:U:122:ARG:HD2  | 2.27        | 0.50     |
| 1:A:1153:C:H2'    | 1:A:1154:G:O4'    | 2.12        | 0.50     |
| 9:I:34:LEU:O      | 9:I:49:GLY:HA3    | 2.12        | 0.50     |
| 12:L:20:ALA:HB1   | 12:L:99:PRO:HD2   | 1.94        | 0.50     |
| 14:N:67:ARG:O     | 14:N:71:ARG:HG3   | 2.12        | 0.50     |
| 15:O:42:ILE:H     | 15:O:42:ILE:HD12  | 1.77        | 0.50     |
| 1:A:2030:A:H4'    | 1:A:2031:A:C8     | 2.47        | 0.49     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:2287:A:N6    | 1:A:2344:U:C2    | 2.80        | 0.49     |
| 1:A:2566:A:H4'   | 1:A:2567:G:O5'   | 2.12        | 0.49     |
| 1:A:654(A):G:N2  | 1:A:654(T):C:C2  | 2.79        | 0.49     |
| 2:B:5:C:O2'      | 2:B:27:C:O2      | 2.30        | 0.49     |
| 5:E:9:ILE:HD11   | 5:E:125:LEU:HG   | 1.94        | 0.49     |
| 13:M:44:LEU:HD22 | 13:M:48:VAL:HG23 | 1.94        | 0.49     |
| 15:O:34:VAL:HG12 | 15:O:36:GLU:HG2  | 1.94        | 0.49     |
| 15:O:41:ARG:CB   | 15:O:41:ARG:NH1  | 2.73        | 0.49     |
| 1:A:2601:C:H2'   | 1:A:2603:G:C8    | 2.47        | 0.49     |
| 7:G:155:SER:OG   | 7:G:156:ALA:N    | 2.45        | 0.49     |
| 12:L:11:LYS:HE2  | 12:L:86:GLY:O    | 2.11        | 0.49     |
| 12:L:69:PHE:CD1  | 12:L:70:PRO:HD2  | 2.46        | 0.49     |
| 14:N:15:ARG:NH1  | 14:N:25:ARG:HH21 | 2.11        | 0.49     |
| 19:S:26:TYR:HB3  | 19:S:92:LEU:HD12 | 1.93        | 0.49     |
| 1:A:1441:G:H2'   | 1:A:1442:G:H8    | 1.77        | 0.49     |
| 1:A:796:C:H2'    | 1:A:797:C:C6     | 2.47        | 0.49     |
| 2:B:78:A:H2'     | 2:B:79:C:O4'     | 2.12        | 0.49     |
| 3:C:175:LEU:HD12 | 3:C:185:VAL:HG21 | 1.93        | 0.49     |
| 8:H:5:LEU:HD23   | 8:H:9:LEU:HD11   | 1.94        | 0.49     |
| 19:S:27:THR:HB   | 19:S:80:ILE:HB   | 1.93        | 0.49     |
| 1:A:1791:A:H5'   | 3:C:206:LEU:HD12 | 1.95        | 0.49     |
| 1:A:229:A:OP1    | 1:A:229:A:H4'    | 2.12        | 0.49     |
| 1:A:2377:A:H2'   | 1:A:2378:A:C8    | 2.48        | 0.49     |
| 6:F:115:ARG:NH2  | 6:F:137:GLU:OE1  | 2.46        | 0.49     |
| 6:F:60:LEU:O     | 6:F:64:THR:HG22  | 2.11        | 0.49     |
| 8:H:2:LYS:HA     | 8:H:20:ASP:HA    | 1.95        | 0.49     |
| 19:S:40:LYS:O    | 19:S:42:ALA:N    | 2.45        | 0.49     |
| 21:U:102:LEU:HB3 | 21:U:104:PHE:HE1 | 1.78        | 0.49     |
| 1:A:1805:U:O2    | 3:C:50:THR:HB    | 2.12        | 0.49     |
| 1:A:2415:G:H4'   | 11:K:67:MET:N    | 2.28        | 0.49     |
| 1:A:404:C:H1'    | 1:A:405:U:OP2    | 2.13        | 0.49     |
| 1:A:813:U:H2'    | 1:A:814:C:C6     | 2.48        | 0.49     |
| 3:C:35:LYS:HZ1   | 3:C:65:ILE:HA    | 1.76        | 0.49     |
| 5:E:132:VAL:HG23 | 5:E:133:ASN:OD1  | 2.12        | 0.49     |
| 9:I:134:ARG:N    | 9:I:135:PRO:HD3  | 2.28        | 0.49     |
| 1:A:2008:C:H2'   | 1:A:2009:G:H8    | 1.78        | 0.49     |
| 1:A:321:G:OP1    | 5:E:135:LYS:NZ   | 2.36        | 0.49     |
| 6:F:110:ALA:HB1  | 6:F:140:ILE:HD12 | 1.94        | 0.49     |
| 15:O:16:ARG:HD3  | 15:O:19:LEU:HD11 | 1.93        | 0.49     |
| 16:P:92:ARG:O    | 16:P:92:ARG:HG2  | 2.13        | 0.49     |
| 1:A:1994:C:P     | 4:D:127:ASP:HB2  | 2.52        | 0.49     |
| 1:A:2527:C:H5''  | 5:E:30:PRO:HB2   | 121.47      | 0.49     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 1:A:2790:A:H2'   | 1:A:2791:C:H5''  | 1.95        | 0.49     |
| 1:A:2795:G:H3'   | 1:A:2797:U:C5'   | 2.43        | 0.49     |
| 3:C:228:PRO:HD3  | 3:C:234:GLY:C    | 2.33        | 0.49     |
| 20:T:47:LYS:HG2  | 20:T:60:PHE:HD1  | 1.76        | 0.49     |
| 25:Y:6:VAL:HG13  | 25:Y:56:VAL:HG13 | 1.93        | 0.49     |
| 1:A:1231:G:H2'   | 1:A:1232:G:C8    | 2.47        | 0.49     |
| 1:A:1533:C:H42   | 1:A:1538:G:H1    | 1.60        | 0.49     |
| 1:A:192:C:O2'    | 1:A:802:A:N3     | 2.42        | 0.49     |
| 1:A:900:A:H3'    | 1:A:901:A:H8     | 1.78        | 0.49     |
| 2:B:15:A:OP1     | 2:B:107:U:O2'    | 2.28        | 0.49     |
| 4:D:70:ALA:O     | 4:D:72:VAL:N     | 2.46        | 0.49     |
| 5:E:178:PRO:HG2  | 5:E:179:GLU:OE2  | 2.13        | 0.49     |
| 1:A:1209:G:O2'   | 1:A:1237:A:N1    | 2.33        | 0.49     |
| 1:A:2364:C:OP1   | 22:V:55:ARG:NH1  | 2.46        | 0.49     |
| 5:E:24:LEU:HD23  | 5:E:115:ALA:HA   | 1.95        | 0.49     |
| 7:G:4:ILE:HG13   | 7:G:6:ARG:NE     | 2.28        | 0.49     |
| 12:L:89:ASN:O    | 12:L:91:GLU:N    | 2.45        | 0.49     |
| 22:V:32:ARG:H    | 22:V:35:ASN:ND2  | 2.11        | 0.49     |
| 6:F:54:GLU:HA    | 6:F:57:ALA:HB3   | 1.94        | 0.49     |
| 8:H:133:HIS:HB2  | 8:H:134:PRO:CD   | 2.43        | 0.49     |
| 1:A:1204:A:H1'   | 1:A:1206:G:C8    | 2.48        | 0.48     |
| 1:A:2037:G:H2'   | 1:A:2038:G:C8    | 2.48        | 0.48     |
| 20:T:47:LYS:HG2  | 20:T:60:PHE:CD1  | 2.48        | 0.48     |
| 1:A:103:A:H8     | 1:A:103:A:O5'    | 1.96        | 0.48     |
| 1:A:1412:A:H2'   | 1:A:1413:G:O4'   | 2.13        | 0.48     |
| 1:A:1803:A:O2'   | 3:C:259:THR:HG21 | 2.14        | 0.48     |
| 1:A:2119:A:N6    | 1:A:2170:A:N7    | 2.61        | 0.48     |
| 1:A:783:A:H2'    | 1:A:784:A:H4'    | 1.94        | 0.48     |
| 5:E:155:LEU:HD12 | 5:E:174:VAL:HG22 | 1.94        | 0.48     |
| 1:A:1777:U:H3    | 1:A:1787:A:H61   | 1.61        | 0.48     |
| 1:A:686:G:N2     | 1:A:788:A:H61    | 2.11        | 0.48     |
| 7:G:41:MET:HG3   | 7:G:54:ARG:HA    | 1.96        | 0.48     |
| 1:A:1190:G:H5'   | 11:K:32:THR:HA   | 1.95        | 0.48     |
| 13:M:2:ARG:HA    | 13:M:5:LYS:HE3   | 1.95        | 0.48     |
| 4:D:181:LEU:HD21 | 15:O:7:ILE:HG23  | 1.95        | 0.48     |
| 19:S:39:ILE:O    | 19:S:43:VAL:HG12 | 2.13        | 0.48     |
| 1:A:263:C:H2'    | 1:A:264:C:O4'    | 2.13        | 0.48     |
| 1:A:626:U:H5''   | 1:A:627:A:H5'    | 1.94        | 0.48     |
| 1:A:78:A:H2'     | 1:A:79:G:C8      | 2.48        | 0.48     |
| 7:G:152:ARG:HH21 | 7:G:153:LYS:HZ1  | 1.61        | 0.48     |
| 13:M:97:VAL:HG22 | 13:M:114:VAL:CG2 | 2.43        | 0.48     |
| 23:W:53:VAL:HB   | 23:W:58:ILE:HD12 | 1.94        | 0.48     |

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| Atom-1          | Atom-2           | Distance(Å) | Clash(Å) |
|-----------------|------------------|-------------|----------|
| 1:A:1062:G:H2'  | 1:A:1063:G:C8    | 2.48        | 0.48     |
| 1:A:2563:U:H1'  | 1:A:2566:A:N6    | 2.29        | 0.48     |
| 1:A:372:G:H1'   | 1:A:373:U:H5     | 1.78        | 0.48     |
| 9:I:4:TYR:O     | 16:P:64:ARG:NH1  | 2.46        | 0.48     |
| 11:K:58:THR:O   | 11:K:61:ARG:CZ   | 2.61        | 0.48     |
| 20:T:81:LYS:NZ  | 20:T:98:VAL:HG11 | 2.28        | 0.48     |
| 1:A:1019:U:HO2' | 1:A:1021:A:H2    | 1.60        | 0.48     |
| 1:A:858:U:O2    | 1:A:2268:A:H2'   | 2.13        | 0.48     |
| 1:A:297:C:H2'   | 1:A:298:G:O4'    | 2.13        | 0.48     |
| 1:A:643:A:N1    | 1:A:2369:A:O2'   | 2.45        | 0.48     |
| 11:K:59:LEU:HA  | 11:K:61:ARG:HE   | 1.76        | 0.48     |
| 25:Y:4:LEU:O    | 25:Y:36:VAL:HA   | 2.13        | 0.48     |
| 1:A:223:A:N1    | 1:A:407:G:O2'    | 2.42        | 0.48     |
| 1:A:2734:A:H5'  | 1:A:2735:G:OP2   | 2.14        | 0.48     |
| 5:E:178:PRO:HB2 | 5:E:201:VAL:HG11 | 1.94        | 0.48     |
| 6:F:81:LYS:O    | 6:F:82:LEU:HB2   | 2.12        | 0.48     |
| 11:K:36:LYS:HB3 | 11:K:40:SER:HB3  | 1.95        | 0.48     |
| 14:N:64:GLU:O   | 14:N:68:GLN:HG3  | 2.14        | 0.48     |
| 1:A:2186:G:H2'  | 1:A:2187:G:H8    | 1.79        | 0.48     |
| 1:A:340:A:H2'   | 1:A:341:G:O4'    | 2.13        | 0.48     |
| 3:C:25:THR:O    | 3:C:27:THR:HG22  | 2.14        | 0.48     |
| 5:E:102:PRO:HB2 | 5:E:105:VAL:HG23 | 1.95        | 0.48     |
| 5:E:197:ASP:OD1 | 5:E:197:ASP:N    | 2.46        | 0.48     |
| 6:F:82:LEU:HD21 | 6:F:88:ILE:HG13  | 1.96        | 0.48     |
| 7:G:86:GLU:OE1  | 7:G:86:GLU:N     | 2.43        | 0.48     |
| 20:T:51:VAL:O   | 20:T:56:PRO:HA   | 2.14        | 0.48     |
| 2:B:13:A:N1     | 2:B:69:G:O2'     | 2.36        | 0.48     |
| 9:I:7:LYS:H     | 9:I:7:LYS:HD2    | 1.79        | 0.48     |
| 26:Z:23:GLU:HG3 | 26:Z:25:TYR:CE2  | 2.49        | 0.48     |
| 1:A:709:U:H3    | 1:A:722:A:H61    | 1.60        | 0.48     |
| 1:A:898:C:H2'   | 1:A:899:A:H5'    | 1.95        | 0.48     |
| 5:E:183:VAL:O   | 5:E:187:VAL:HG23 | 2.13        | 0.48     |
| 8:H:13:GLY:HA3  | 8:H:17:GLN:CD    | 2.33        | 0.48     |
| 21:U:52:SER:O   | 21:U:54:HIS:N    | 2.46        | 0.48     |
| 21:U:91:LEU:CD1 | 21:U:96:VAL:HG21 | 2.43        | 0.48     |
| 1:A:2050:C:N4   | 1:A:2051:A:N1    | 2.62        | 0.47     |
| 1:A:2283:C:H2'  | 1:A:2284:C:O4'   | 2.13        | 0.47     |
| 1:A:2331:G:O2'  | 22:V:43:THR:HG22 | 2.14        | 0.47     |
| 1:A:724:U:H2'   | 1:A:725:G:O4'    | 2.13        | 0.47     |
| 1:A:848:G:H2'   | 1:A:849:A:C8     | 2.49        | 0.47     |
| 1:A:870:A:OP1   | 12:L:6:ARG:NE    | 2.47        | 0.47     |
| 2:B:104:A:H2'   | 2:B:105:G:O4'    | 2.14        | 0.47     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 5:E:167:ALA:HB1  | 5:E:173:VAL:HG11 | 1.95        | 0.47     |
| 7:G:154:PRO:HD3  | 7:G:162:ILE:H    | 1.77        | 0.47     |
| 4:D:13:ARG:HD2   | 11:K:61:ARG:CD   | 122.65      | 0.47     |
| 15:O:41:ARG:CB   | 15:O:41:ARG:HH11 | 2.27        | 0.47     |
| 19:S:83:VAL:HG11 | 19:S:87:GLN:HB2  | 1.96        | 0.47     |
| 2:B:43:C:H5'     | 26:Z:1:MET:HA    | 1.95        | 0.47     |
| 6:F:145:THR:O    | 6:F:147:ASP:N    | 2.47        | 0.47     |
| 8:H:128:LEU:HD13 | 8:H:128:LEU:HA   | 1.56        | 0.47     |
| 8:H:49:ALA:O     | 8:H:52:ARG:HG2   | 2.14        | 0.47     |
| 11:K:127:ALA:HB3 | 11:K:130:PHE:CZ  | 2.49        | 0.47     |
| 1:A:297:C:H5''   | 20:T:85:VAL:HG21 | 1.95        | 0.47     |
| 24:X:41:ILE:HD11 | 24:X:44:LEU:HD12 | 1.96        | 0.47     |
| 1:A:2328:A:H2'   | 1:A:2329:G:C8    | 2.49        | 0.47     |
| 1:A:99:U:H4'     | 1:A:101:G:O5'    | 2.14        | 0.47     |
| 12:L:136:ALA:C   | 12:L:138:ASP:H   | 2.18        | 0.47     |
| 15:O:64:ARG:HD2  | 15:O:73:GLU:OE1  | 2.14        | 0.47     |
| 1:A:1754:C:P     | 15:O:96:ARG:HH12 | 2.37        | 0.47     |
| 23:W:91:LYS:O    | 23:W:94:LEU:N    | 2.36        | 0.47     |
| 1:A:1028:A:N6    | 1:A:1125:G:H2'   | 2.29        | 0.47     |
| 1:A:1794:U:H2'   | 1:A:1795:C:C6    | 2.49        | 0.47     |
| 1:A:1952:A:C2    | 10:J:22:ILE:HG23 | 2.50        | 0.47     |
| 1:A:205:G:H1'    | 1:A:206:U:OP2    | 2.14        | 0.47     |
| 1:A:611:C:H2'    | 1:A:612:G:H8     | 1.80        | 0.47     |
| 4:D:21:VAL:CG2   | 4:D:22:PRO:N     | 2.74        | 0.47     |
| 5:E:6:VAL:CG1    | 5:E:24:LEU:HD23  | 2.43        | 0.47     |
| 6:F:3:LEU:HD11   | 26:Z:25:TYR:CE1  | 2.48        | 0.47     |
| 8:H:55:ALA:HA    | 8:H:58:LEU:HB2   | 1.94        | 0.47     |
| 16:P:97:ASP:OD2  | 16:P:101:ARG:NH1 | 2.48        | 0.47     |
| 1:A:2327:A:H2'   | 1:A:2328:A:C8    | 2.49        | 0.47     |
| 1:A:2823:A:OP1   | 4:D:113:PHE:HB2  | 2.15        | 0.47     |
| 1:A:581:C:H2'    | 1:A:582:G:H8     | 1.78        | 0.47     |
| 1:A:662:G:H5'    | 11:K:15:ARG:HA   | 1.95        | 0.47     |
| 4:D:37:ARG:NE    | 4:D:37:ARG:HA    | 2.29        | 0.47     |
| 12:L:63:LYS:HG2  | 12:L:65:PHE:CE1  | 2.50        | 0.47     |
| 20:T:21:LYS:HG3  | 20:T:22:GLY:N    | 2.30        | 0.47     |
| 1:A:1407:C:H42   | 1:A:1595:G:H1    | 1.62        | 0.47     |
| 1:A:1667:G:O2'   | 1:A:1991:U:O4    | 2.32        | 0.47     |
| 1:A:2747:G:N2    | 1:A:2757:A:H62   | 2.11        | 0.47     |
| 1:A:706:A:H2'    | 1:A:707:G:O4'    | 2.14        | 0.47     |
| 8:H:98:ALA:HA    | 8:H:109:ILE:HD11 | 1.97        | 0.47     |
| 18:R:63:ASP:OD1  | 18:R:63:ASP:N    | 2.48        | 0.47     |
| 1:A:2086:U:H2'   | 1:A:2087:G:C8    | 2.49        | 0.47     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:A:2512:C:H2'    | 1:A:2513:G:O4'    | 2.14        | 0.47     |
| 1:A:2698:U:H2'    | 1:A:2699:C:C6     | 2.49        | 0.47     |
| 1:A:740:U:H2'     | 1:A:741:G:C8      | 2.50        | 0.47     |
| 4:D:73:GLU:HG3    | 4:D:74:PRO:HD2    | 1.95        | 0.47     |
| 1:A:2849:U:H4'    | 1:A:2868:A:C2     | 2.50        | 0.47     |
| 1:A:576:U:OP1     | 1:A:2503:A:OP1    | 2.33        | 0.47     |
| 1:A:764:A:H5'     | 3:C:210:GLY:HA2   | 1.95        | 0.47     |
| 7:G:152:ARG:HG3   | 7:G:153:LYS:CD    | 2.44        | 0.47     |
| 8:H:88:ILE:HG12   | 8:H:122:GLU:H     | 1.80        | 0.47     |
| 13:M:1:MET:HB3    | 13:M:2:ARG:H      | 1.35        | 0.47     |
| 15:O:123:GLN:O    | 15:O:125:ARG:N    | 2.48        | 0.47     |
| 21:U:141:VAL:HA   | 21:U:144:LEU:HD23 | 1.96        | 0.47     |
| 1:A:1292:U:H2'    | 1:A:1293:C:C6     | 2.50        | 0.47     |
| 1:A:1348:G:H2'    | 1:A:1349:A:H5''   | 1.97        | 0.47     |
| 1:A:2150:U:H2'    | 1:A:2151:G:C8     | 2.50        | 0.47     |
| 1:A:2116:G:H1     | 1:A:2162:G:P      | 2.38        | 0.47     |
| 1:A:2689:U:H4'    | 1:A:2690:C:O5'    | 2.13        | 0.47     |
| 1:A:2779:U:O2'    | 1:A:2781:A:C5     | 2.66        | 0.47     |
| 1:A:628:G:O2'     | 1:A:651:G:O2'     | 2.17        | 0.47     |
| 4:D:95:ILE:H      | 4:D:95:ILE:HD12   | 1.80        | 0.47     |
| 5:E:133:ASN:HA    | 5:E:162:LEU:HD22  | 1.96        | 0.47     |
| 5:E:62:ARG:HB3    | 5:E:62:ARG:CZ     | 2.45        | 0.47     |
| 7:G:27:LYS:HA     | 7:G:32:GLU:HA     | 1.96        | 0.47     |
| 1:A:1142(A):A:H4' | 9:I:25:ARG:HH22   | 1.80        | 0.47     |
| 1:A:389:G:N1      | 11:K:70:GLN:HB3   | 2.30        | 0.47     |
| 20:T:76:CYS:HB2   | 20:T:101:LYS:HG3  | 1.96        | 0.47     |
| 1:A:2735:G:H2'    | 1:A:2736:G:C8     | 2.48        | 0.47     |
| 1:A:709:U:H2'     | 1:A:710:G:C8      | 2.50        | 0.47     |
| 1:A:389:G:H1      | 11:K:70:GLN:HB3   | 1.79        | 0.47     |
| 2:B:8:U:O3'       | 14:N:25:ARG:NH2   | 2.47        | 0.47     |
| 14:N:56:LEU:O     | 14:N:58:LEU:N     | 2.48        | 0.47     |
| 17:Q:24:LYS:HG3   | 17:Q:92:THR:HG23  | 1.97        | 0.47     |
| 19:S:49:VAL:HG13  | 19:S:83:VAL:HG13  | 1.96        | 0.47     |
| 23:W:76:ARG:H     | 23:W:76:ARG:HD2   | 1.80        | 0.47     |
| 1:A:117:G:OP2     | 1:A:119:A:O2'     | 2.22        | 0.47     |
| 1:A:1359:A:C6     | 1:A:1373:A:C5     | 3.03        | 0.47     |
| 1:A:2378:A:O5'    | 1:A:2378:A:H8     | 1.99        | 0.47     |
| 1:A:2610:C:H4'    | 1:A:2611:U:OP2    | 2.14        | 0.47     |
| 1:A:2645:G:C3'    | 1:A:2646:C:H5'    | 2.45        | 0.47     |
| 1:A:2867:G:O2'    | 1:A:2868:A:P      | 2.73        | 0.47     |
| 3:C:118:VAL:HG22  | 3:C:119:ALA:N     | 2.29        | 0.47     |
| 3:C:211:ARG:HD2   | 3:C:214:TRP:CZ3   | 2.50        | 0.47     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 8:H:9:LEU:O      | 8:H:10:GLU:HG3   | 2.15        | 0.47     |
| 14:N:48:LEU:HD23 | 14:N:82:ILE:HD11 | 1.96        | 0.47     |
| 1:A:2387:U:O2'   | 22:V:19:LYS:NZ   | 2.48        | 0.47     |
| 1:A:1287:A:N7    | 13:M:107:ASP:HB2 | 2.30        | 0.46     |
| 1:A:1796:U:H2'   | 1:A:1797:C:C6    | 2.50        | 0.46     |
| 1:A:2562:U:O2'   | 10:J:23:ARG:NH1  | 2.44        | 0.46     |
| 1:A:50:U:H3'     | 1:A:51:G:H5'     | 1.97        | 0.46     |
| 1:A:639:U:H2'    | 1:A:640:C:C6     | 2.49        | 0.46     |
| 2:B:16:G:H1      | 2:B:68:C:N4      | 2.13        | 0.46     |
| 3:C:12:SER:O     | 3:C:16:MET:HB2   | 2.14        | 0.46     |
| 3:C:43:ARG:HH11  | 3:C:44:ASN:CG    | 2.16        | 0.46     |
| 11:K:83:VAL:HG12 | 11:K:114:ILE:HA  | 1.97        | 0.46     |
| 15:O:20:PRO:HD2  | 15:O:86:ILE:HG23 | 1.97        | 0.46     |
| 1:A:2294:C:H2'   | 1:A:2295:C:C6    | 2.50        | 0.46     |
| 4:D:186:GLY:O    | 4:D:188:VAL:N    | 2.48        | 0.46     |
| 1:A:2444:G:P     | 5:E:68:LYS:HE3   | 2.55        | 0.46     |
| 5:E:6:VAL:HG11   | 5:E:24:LEU:HD23  | 1.97        | 0.46     |
| 7:G:153:LYS:HB3  | 7:G:162:ILE:H    | 1.80        | 0.46     |
| 8:H:40:THR:O     | 8:H:44:LEU:N     | 2.44        | 0.46     |
| 15:O:16:ARG:HE   | 15:O:19:LEU:HD21 | 1.80        | 0.46     |
| 16:P:8:VAL:HG23  | 16:P:11:ARG:HH21 | 1.80        | 0.46     |
| 18:R:23:LEU:O    | 18:R:27:LYS:HD2  | 2.14        | 0.46     |
| 20:T:89:PHE:O    | 20:T:90:LEU:HD13 | 2.15        | 0.46     |
| 1:A:1007:C:OP1   | 9:I:37:LYS:NZ    | 2.41        | 0.46     |
| 1:A:1801:G:OP2   | 3:C:154:LYS:HE2  | 2.16        | 0.46     |
| 1:A:2271:G:OP1   | 22:V:18:ALA:HB1  | 2.15        | 0.46     |
| 1:A:2758:A:H2'   | 1:A:2759:G:O4'   | 2.15        | 0.46     |
| 1:A:222:A:H3'    | 1:A:421:U:H5''   | 1.96        | 0.46     |
| 3:C:70:TRP:CD2   | 3:C:150:LYS:HD2  | 2.49        | 0.46     |
| 1:A:2680:C:OP2   | 4:D:111:ARG:NH2  | 2.48        | 0.46     |
| 6:F:22:ARG:HH22  | 6:F:175:LEU:HD21 | 1.80        | 0.46     |
| 8:H:104:GLN:C    | 8:H:105:HIS:HD1  | 2.18        | 0.46     |
| 1:A:1278:A:H4'   | 13:M:34:ILE:HD12 | 1.96        | 0.46     |
| 14:N:78:LEU:HD11 | 14:N:107:GLU:O   | 2.15        | 0.46     |
| 23:W:89:GLU:HA   | 23:W:93:GLU:HB2  | 1.96        | 0.46     |
| 1:A:1936:A:H61   | 1:A:1963:U:H3    | 1.63        | 0.46     |
| 1:A:2623:G:OP1   | 1:A:2826:A:O2'   | 2.22        | 0.46     |
| 10:J:76:ALA:HB3  | 15:O:75:ILE:HB   | 1.97        | 0.46     |
| 1:A:1678:G:N2    | 1:A:1989:G:H22   | 2.13        | 0.46     |
| 1:A:581:C:H2'    | 1:A:582:G:C8     | 2.50        | 0.46     |
| 5:E:126:VAL:HG11 | 5:E:142:TRP:HH2  | 1.80        | 0.46     |
| 11:K:124:LYS:HA  | 11:K:143:GLY:O   | 2.16        | 0.46     |

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| Atom-1           | Atom-2            | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 19:S:55:ASN:HB2  | 19:S:80:ILE:HG23  | 1.97        | 0.46     |
| 21:U:157:LEU:HA  | 21:U:158:PRO:HD2  | 1.70        | 0.46     |
| 1:A:2676:C:O2    | 1:A:2732:G:N2     | 2.48        | 0.46     |
| 1:A:407:G:H2'    | 1:A:408:G:H8      | 1.81        | 0.46     |
| 1:A:593:G:H1     | 1:A:664:C:H42     | 1.63        | 0.46     |
| 6:F:98:ARG:O     | 6:F:101:ILE:HG13  | 2.16        | 0.46     |
| 8:H:113:ARG:HG3  | 8:H:131:LYS:HZ2   | 1.80        | 0.46     |
| 1:A:2818:G:P     | 13:M:42:LYS:HZ3   | 2.39        | 0.46     |
| 14:N:61:ASN:O    | 14:N:65:VAL:HG23  | 2.14        | 0.46     |
| 1:A:1416:G:H2'   | 1:A:1417:C:C6     | 2.51        | 0.46     |
| 1:A:1791:A:N6    | 1:A:1828:G:O2'    | 2.36        | 0.46     |
| 1:A:922:U:H2'    | 1:A:923:C:C6      | 2.51        | 0.46     |
| 1:A:1819:A:H2'   | 3:C:178:PRO:HB2   | 1.98        | 0.46     |
| 8:H:29:TYR:CD2   | 8:H:30:LEU:HD23   | 2.51        | 0.46     |
| 14:N:83:LYS:O    | 14:N:109:GLY:HA3  | 2.15        | 0.46     |
| 18:R:86:LEU:O    | 18:R:94:ASP:N     | 2.44        | 0.46     |
| 20:T:17:SER:OG   | 20:T:71:LYS:HD2   | 2.16        | 0.46     |
| 21:U:53:ILE:HG22 | 21:U:71:VAL:HG22  | 1.98        | 0.46     |
| 1:A:2696:U:H2'   | 1:A:2697:G:C8     | 2.50        | 0.46     |
| 1:A:811:U:OP2    | 11:K:29:LYS:N     | 2.42        | 0.46     |
| 7:G:87:LEU:HA    | 7:G:163:TYR:O     | 2.16        | 0.46     |
| 8:H:76:THR:OG1   | 8:H:139:GLN:OE1   | 2.34        | 0.46     |
| 1:A:1593:G:H2'   | 1:A:1594:G:C8     | 2.51        | 0.46     |
| 1:A:1773:A:H2'   | 1:A:1774:C:O4'    | 2.16        | 0.46     |
| 1:A:1812:A:H2'   | 1:A:1813:G:C8     | 2.51        | 0.46     |
| 1:A:2154:G:H2'   | 1:A:2155:G:H8     | 1.79        | 0.46     |
| 1:A:503:A:H4'    | 1:A:504:U:O5'     | 2.16        | 0.46     |
| 7:G:115:VAL:HG11 | 7:G:148:ILE:HD11  | 1.98        | 0.46     |
| 1:A:2751:G:N7    | 7:G:2:SER:HB3     | 2.31        | 0.46     |
| 7:G:85:LYS:HA    | 7:G:85:LYS:HD2    | 1.85        | 0.46     |
| 8:H:112:LYS:H    | 8:H:112:LYS:HG2   | 1.50        | 0.46     |
| 12:L:2:LEU:HD23  | 12:L:2:LEU:H      | 1.81        | 0.46     |
| 21:U:23:LYS:HB3  | 21:U:38:TYR:CD1   | 2.51        | 0.46     |
| 1:A:1045:A:O2'   | 1:A:1046:A:OP2    | 2.31        | 0.46     |
| 1:A:1047:G:H2'   | 1:A:1110:G:N1     | 2.31        | 0.46     |
| 1:A:2567:G:H2'   | 1:A:2568:C:C6     | 2.51        | 0.46     |
| 3:C:68:LYS:HD2   | 3:C:70:TRP:CZ2    | 2.51        | 0.46     |
| 4:D:63:LEU:HD12  | 4:D:64:LYS:N      | 2.30        | 0.46     |
| 7:G:103:LEU:HD13 | 7:G:131:VAL:HG11  | 1.97        | 0.46     |
| 10:J:31:LYS:HB3  | 10:J:32:TYR:CD2   | 2.51        | 0.46     |
| 11:K:6:LEU:HB3   | 11:K:7:ARG:H      | 1.55        | 0.46     |
| 12:L:104:PHE:HE2 | 12:L:125:LEU:HD11 | 1.80        | 0.46     |

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| Atom-1            | Atom-2           | Distance(Å) | Clash(Å) |
|-------------------|------------------|-------------|----------|
| 14:N:24:LEU:HB2   | 14:N:85:VAL:HG12 | 1.97        | 0.46     |
| 16:P:69:CYS:HB3   | 16:P:106:PHE:HZ  | 1.81        | 0.46     |
| 17:Q:51:VAL:HG12  | 17:Q:53:GLU:H    | 1.80        | 0.46     |
| 23:W:73:LEU:HB3   | 23:W:90:ILE:HG23 | 1.97        | 0.46     |
| 1:A:1203:G:H3'    | 1:A:1204:A:H5''  | 1.98        | 0.45     |
| 1:A:1336:A:H2'    | 1:A:1337:G:C8    | 2.51        | 0.45     |
| 1:A:2645:G:H3'    | 1:A:2646:C:H5'   | 1.97        | 0.45     |
| 2:B:15:A:H1'      | 2:B:109:G:N9     | 2.31        | 0.45     |
| 7:G:120:GLY:HA3   | 7:G:140:LYS:NZ   | 2.31        | 0.45     |
| 11:K:101:VAL:HG23 | 11:K:107:LYS:H   | 1.81        | 0.45     |
| 12:L:29:PHE:N     | 12:L:105:GLU:OE2 | 2.40        | 0.45     |
| 13:M:37:THR:OG1   | 13:M:40:LYS:HG3  | 2.17        | 0.45     |
| 1:A:2019:A:H4'    | 16:P:34:LYS:HD2  | 1.99        | 0.45     |
| 1:A:1228:G:OP1    | 16:P:13:LYS:HG2  | 2.15        | 0.45     |
| 1:A:622:G:H2'     | 1:A:623:G:H8     | 1.81        | 0.45     |
| 11:K:77:ARG:HB2   | 11:K:78:PRO:HD2  | 1.98        | 0.45     |
| 15:O:26:ASP:HB2   | 15:O:90:GLN:O    | 2.16        | 0.45     |
| 1:A:1469:A:H2'    | 1:A:1470:G:O4'   | 2.16        | 0.45     |
| 1:A:2116:G:N1     | 1:A:2162:G:OP1   | 2.50        | 0.45     |
| 1:A:2543:G:H2'    | 1:A:2544:G:C8    | 2.51        | 0.45     |
| 1:A:468:G:H5''    | 5:E:60:SER:HB2   | 1.98        | 0.45     |
| 3:C:121:PRO:HB3   | 3:C:135:PHE:CE2  | 2.52        | 0.45     |
| 13:M:33:ARG:HG2   | 13:M:34:ILE:N    | 2.30        | 0.45     |
| 1:A:1210:A:H4'    | 1:A:1211:U:O5'   | 2.16        | 0.45     |
| 1:A:1220:A:H5'    | 1:A:1221:C:OP2   | 2.16        | 0.45     |
| 1:A:1527:G:H2'    | 1:A:1543:A:N1    | 2.30        | 0.45     |
| 1:A:2307:G:H1'    | 1:A:2308:G:C2    | 2.52        | 0.45     |
| 1:A:2695:C:H2'    | 1:A:2696:U:C6    | 2.52        | 0.45     |
| 1:A:898:C:C2'     | 1:A:899:A:H5'    | 2.47        | 0.45     |
| 3:C:118:VAL:HG22  | 3:C:119:ALA:H    | 1.82        | 0.45     |
| 3:C:30:GLU:HG3    | 3:C:63:ARG:CZ    | 2.47        | 0.45     |
| 7:G:170:ARG:HB3   | 7:G:171:LEU:H    | 1.52        | 0.45     |
| 14:N:16:ASN:HA    | 14:N:19:LYS:HD3  | 1.99        | 0.45     |
| 13:M:103:ARG:NH1  | 18:R:40:ASN:OD1  | 2.50        | 0.45     |
| 1:A:1101:U:H2'    | 1:A:1102:C:C6    | 2.52        | 0.45     |
| 1:A:1860:G:H2'    | 1:A:1861:G:C8    | 2.52        | 0.45     |
| 1:A:2245:U:C5'    | 1:A:2246:G:H5'   | 2.46        | 0.45     |
| 1:A:2291:U:H2'    | 1:A:2292:C:C6    | 2.52        | 0.45     |
| 1:A:2469:A:H5''   | 1:A:2470:G:H8    | 1.81        | 0.45     |
| 1:A:443:A:H3'     | 5:E:45:ARG:HH12  | 1.82        | 0.45     |
| 7:G:153:LYS:HG3   | 7:G:161:GLY:HA2  | 1.97        | 0.45     |
| 10:J:48:PRO:O     | 10:J:49:ARG:HG2  | 2.17        | 0.45     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 11:K:88:LEU:HD12 | 11:K:95:VAL:HG11 | 1.99        | 0.45     |
| 21:U:118:GLN:O   | 21:U:120:ILE:N   | 2.46        | 0.45     |
| 1:A:1220:A:OP2   | 16:P:19:LYS:NZ   | 2.35        | 0.45     |
| 1:A:195:A:H5''   | 1:A:196:A:O5'    | 2.16        | 0.45     |
| 1:A:2692:C:H2'   | 1:A:2693:A:H8    | 1.82        | 0.45     |
| 1:A:1637:A:H4'   | 1:A:2711:A:O2'   | 2.17        | 0.45     |
| 1:A:627:A:H4'    | 1:A:628:G:H5'    | 1.99        | 0.45     |
| 1:A:774:A:H2     | 1:A:787:U:O2'    | 2.00        | 0.45     |
| 6:F:106:LEU:HA   | 6:F:110:ALA:HB3  | 1.98        | 0.45     |
| 9:I:19:GLU:HB2   | 9:I:56:ASN:HD22  | 1.80        | 0.45     |
| 11:K:18:ARG:HD2  | 11:K:27:HIS:HD2  | 1.81        | 0.45     |
| 4:D:111:ARG:HA   | 13:M:1:MET:SD    | 2.57        | 0.45     |
| 13:M:42:LYS:HA   | 13:M:45:ARG:HD2  | 1.98        | 0.45     |
| 14:N:10:ARG:O    | 14:N:14:VAL:HG12 | 2.17        | 0.45     |
| 1:A:2022:U:O2'   | 1:A:2617:C:H5'   | 2.16        | 0.45     |
| 1:A:307:G:N2     | 1:A:330:A:H62    | 2.14        | 0.45     |
| 1:A:479:A:N3     | 1:A:481:G:H5''   | 2.32        | 0.45     |
| 2:B:89(A):A:O5'  | 2:B:89(A):A:H8   | 2.00        | 0.45     |
| 3:C:76:PRO:HB2   | 3:C:116:GLN:OE1  | 2.17        | 0.45     |
| 6:F:10:LYS:O     | 6:F:14:GLU:HB3   | 2.17        | 0.45     |
| 8:H:101:LEU:HD22 | 8:H:107:VAL:HB   | 1.98        | 0.45     |
| 1:A:1012:U:O4    | 9:I:25:ARG:HA    | 2.16        | 0.45     |
| 12:L:111:GLU:C   | 12:L:113:GLN:H   | 2.19        | 0.45     |
| 13:M:78:LYS:HE2  | 13:M:83:ILE:HD11 | 1.98        | 0.45     |
| 20:T:68:HIS:CE1  | 20:T:70:SER:HB3  | 2.52        | 0.45     |
| 20:T:90:LEU:HB2  | 20:T:91:GLU:H    | 1.63        | 0.45     |
| 26:Z:10:VAL:HA   | 26:Z:11:PRO:HD2  | 1.75        | 0.45     |
| 1:A:1029:A:OP1   | 12:L:128:LYS:HE3 | 2.17        | 0.45     |
| 1:A:1827:C:OP2   | 3:C:222:ARG:NH1  | 2.44        | 0.45     |
| 1:A:2308:G:C6    | 1:A:2311:A:N1    | 2.85        | 0.45     |
| 1:A:345:A:H5''   | 1:A:346:A:OP1    | 2.17        | 0.45     |
| 1:A:463:G:N2     | 1:A:466:A:OP2    | 2.48        | 0.45     |
| 1:A:57:C:H2'     | 1:A:58:G:O4'     | 2.17        | 0.45     |
| 4:D:46:ALA:HB2   | 4:D:82:ARG:HA    | 1.98        | 0.45     |
| 7:G:125:VAL:HG13 | 7:G:126:PRO:HB3  | 1.99        | 0.45     |
| 1:A:805:G:OP2    | 11:K:41:ARG:HG2  | 2.17        | 0.45     |
| 21:U:53:ILE:H    | 21:U:71:VAL:CG1  | 2.30        | 0.45     |
| 24:X:41:ILE:HD11 | 24:X:44:LEU:HB2  | 1.98        | 0.45     |
| 1:A:856:C:HO2'   | 1:A:857:C:P      | 2.39        | 0.45     |
| 5:E:45:ARG:HH11  | 5:E:45:ARG:CG    | 2.29        | 0.45     |
| 10:J:22:ILE:HG12 | 10:J:41:ALA:HA   | 1.98        | 0.45     |
| 21:U:181:GLU:HB3 | 21:U:182:LYS:HD3 | 1.98        | 0.45     |

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| Atom-1           | Atom-2            | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:A:270:A:OP2    | 1:A:270(Y):G:N1   | 2.38        | 0.45     |
| 2:B:31:C:N4      | 2:B:51:G:H1       | 2.15        | 0.45     |
| 3:C:85:ASP:HA    | 3:C:86:PRO:HD2    | 1.72        | 0.45     |
| 4:D:107:THR:O    | 4:D:190:GLY:HA2   | 2.17        | 0.45     |
| 5:E:161:GLU:OE2  | 5:E:164:ARG:NH1   | 2.50        | 0.45     |
| 6:F:102:PHE:O    | 6:F:106:LEU:N     | 2.50        | 0.45     |
| 1:A:2311:A:C8    | 6:F:88:ILE:HD11   | 2.52        | 0.45     |
| 7:G:52:VAL:HG21  | 7:G:69:ARG:HA     | 1.98        | 0.45     |
| 8:H:14:ASP:N     | 8:H:14:ASP:OD1    | 2.50        | 0.45     |
| 1:A:2712:U:OP1   | 1:A:2714:G:H4'    | 2.17        | 0.44     |
| 3:C:105:ILE:HA   | 3:C:105:ILE:HD12  | 1.63        | 0.44     |
| 10:J:111:PHE:HB3 | 10:J:114:ILE:HG13 | 1.98        | 0.44     |
| 13:M:29:LEU:HA   | 13:M:29:LEU:HD12  | 1.74        | 0.44     |
| 13:M:28:LEU:HD12 | 13:M:48:VAL:HG11  | 1.99        | 0.44     |
| 20:T:42:VAL:HG12 | 20:T:65:ALA:HB3   | 1.99        | 0.44     |
| 23:W:83:GLU:N    | 23:W:83:GLU:OE2   | 2.49        | 0.44     |
| 1:A:1337:G:H2'   | 1:A:1338:G:H8     | 1.81        | 0.44     |
| 1:A:1664:A:H61   | 1:A:1996:C:H42    | 1.65        | 0.44     |
| 1:A:188:G:H5'    | 23:W:14:VAL:HG21  | 1.99        | 0.44     |
| 1:A:77:C:H5''    | 24:X:10:LEU:HD11  | 1.97        | 0.44     |
| 7:G:109:PHE:CZ   | 7:G:152:ARG:HG2   | 2.53        | 0.44     |
| 9:I:114:ARG:O    | 9:I:115:ARG:HB3   | 2.17        | 0.44     |
| 10:J:87:ILE:HD12 | 10:J:91:LEU:HD12  | 1.99        | 0.44     |
| 12:L:12:GLN:HE21 | 12:L:72:LYS:HD3   | 1.82        | 0.44     |
| 1:A:2537:U:H2'   | 1:A:2538:C:C6     | 2.53        | 0.44     |
| 1:A:300:A:H1'    | 1:A:319:C:H1'     | 1.99        | 0.44     |
| 1:A:512:G:H4'    | 1:A:513:A:O5'     | 2.18        | 0.44     |
| 9:I:116:LEU:HD23 | 9:I:116:LEU:HA    | 1.78        | 0.44     |
| 1:A:144:C:H2'    | 1:A:145:G:H8      | 1.82        | 0.44     |
| 1:A:1537:C:H2'   | 1:A:1538:G:C8     | 2.52        | 0.44     |
| 3:C:49:ILE:CD1   | 3:C:52:ARG:HA     | 2.47        | 0.44     |
| 6:F:51:ARG:O     | 6:F:53:LEU:N      | 2.48        | 0.44     |
| 6:F:57:ALA:HB1   | 6:F:68:PRO:HG2    | 1.99        | 0.44     |
| 11:K:140:ALA:O   | 11:K:141:ALA:HB2  | 2.17        | 0.44     |
| 15:O:36:GLU:HG3  | 15:O:41:ARG:CD    | 2.45        | 0.44     |
| 16:P:65:ILE:HG12 | 16:P:96:ALA:CB    | 2.47        | 0.44     |
| 19:S:53:LYS:NZ   | 19:S:55:ASN:HD21  | 2.15        | 0.44     |
| 21:U:103:ARG:HD3 | 21:U:136:PHE:CD2  | 2.53        | 0.44     |
| 1:A:2821:A:OP2   | 1:A:2822:G:OP2    | 2.36        | 0.44     |
| 2:B:24:G:H1'     | 2:B:27:C:N4       | 2.33        | 0.44     |
| 6:F:37:VAL:O     | 6:F:94:LEU:HG     | 2.17        | 0.44     |
| 14:N:11:LYS:HG3  | 14:N:91:PRO:HD3   | 1.98        | 0.44     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 17:Q:16:PRO:HB3  | 17:Q:97:LYS:O    | 2.17        | 0.44     |
| 1:A:1007:C:H5''  | 9:I:35:ARG:HH11  | 1.81        | 0.44     |
| 1:A:1085:A:HO2'  | 1:A:1086:A:P     | 2.40        | 0.44     |
| 1:A:1534:G:N3    | 1:A:1534:G:H2'   | 2.32        | 0.44     |
| 1:A:748:G:C8     | 18:R:89:ALA:HB1  | 2.53        | 0.44     |
| 3:C:34:VAL:HG22  | 3:C:35:LYS:HG3   | 2.00        | 0.44     |
| 3:C:70:TRP:HZ3   | 3:C:146:GLU:OE2  | 2.01        | 0.44     |
| 8:H:93:THR:H     | 8:H:96:ASP:HB2   | 1.82        | 0.44     |
| 10:J:22:ILE:HA   | 10:J:22:ILE:HD13 | 1.77        | 0.44     |
| 5:E:117:ARG:HH12 | 11:K:1:MET:N     | 2.16        | 0.44     |
| 11:K:37:GLY:O    | 11:K:40:SER:OG   | 2.27        | 0.44     |
| 17:Q:49:THR:HB   | 17:Q:50:PRO:HD2  | 1.99        | 0.44     |
| 24:X:49:LYS:O    | 24:X:53:LEU:HB2  | 2.18        | 0.44     |
| 1:A:271(B):G:H2' | 1:A:421:U:OP2    | 2.17        | 0.44     |
| 5:E:9:ILE:HA     | 5:E:10:PRO:HD3   | 1.89        | 0.44     |
| 6:F:171:ALA:O    | 6:F:175:LEU:HG   | 2.18        | 0.44     |
| 7:G:28:GLY:HA3   | 7:G:79:VAL:HB    | 2.00        | 0.44     |
| 1:A:2563:U:H4'   | 10:J:28:SER:HA   | 2.00        | 0.44     |
| 14:N:19:LYS:O    | 14:N:20:ARG:HB3  | 2.17        | 0.44     |
| 17:Q:35:LEU:CD2  | 17:Q:57:VAL:HG22 | 2.47        | 0.44     |
| 21:U:102:LEU:HB3 | 21:U:104:PHE:CE1 | 2.52        | 0.44     |
| 21:U:148:ASP:OD1 | 21:U:149:SER:N   | 2.50        | 0.44     |
| 1:A:1331:A:O2'   | 1:A:1332:G:H8    | 2.00        | 0.44     |
| 1:A:1543:A:H2    | 1:A:1545:A:N7    | 2.16        | 0.44     |
| 1:A:807:U:O2'    | 1:A:2060:A:N1    | 2.46        | 0.44     |
| 6:F:95:ARG:O     | 6:F:99:MET:HG2   | 2.18        | 0.44     |
| 7:G:123:PHE:O    | 7:G:125:VAL:HG23 | 2.18        | 0.44     |
| 1:A:558:G:OP1    | 9:I:111:PRO:HD2  | 2.18        | 0.44     |
| 13:M:54:LEU:HD23 | 13:M:66:VAL:HG23 | 1.98        | 0.44     |
| 15:O:107:ASP:O   | 15:O:111:ARG:NH1 | 2.51        | 0.44     |
| 19:S:57:LEU:HD11 | 19:S:78:LYS:HD2  | 1.99        | 0.44     |
| 19:S:87:GLN:O    | 19:S:88:LYS:HG3  | 2.18        | 0.44     |
| 1:A:2396:G:O5'   | 23:W:25:LYS:HE2  | 2.18        | 0.44     |
| 1:A:1178:C:H2'   | 1:A:1179:C:C6    | 2.53        | 0.44     |
| 1:A:134:C:H2'    | 1:A:135:G:C8     | 2.53        | 0.44     |
| 1:A:191:A:H2'    | 1:A:192:C:C6     | 2.52        | 0.44     |
| 1:A:2556:C:H2'   | 1:A:2557:G:O4'   | 2.17        | 0.44     |
| 1:A:859:G:O2'    | 1:A:860:U:O2     | 2.20        | 0.44     |
| 3:C:65:ILE:H     | 3:C:65:ILE:HD13  | 1.82        | 0.44     |
| 4:D:143:ASN:HD22 | 4:D:147:PRO:HD3  | 1.83        | 0.44     |
| 6:F:95:ARG:C     | 6:F:99:MET:HG2   | 2.38        | 0.44     |
| 8:H:64:GLU:O     | 8:H:67:ARG:NH2   | 2.51        | 0.44     |

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| Atom-1           | Atom-2            | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 13:M:27:SER:HB3  | 13:M:34:ILE:HD11  | 2.00        | 0.44     |
| 21:U:29:TYR:CE2  | 21:U:87:ASP:HB3   | 2.53        | 0.44     |
| 1:A:1363:C:H2'   | 1:A:1364:G:H8     | 1.83        | 0.43     |
| 1:A:1543:A:N3    | 1:A:1545:A:O4'    | 2.51        | 0.43     |
| 1:A:210:C:H2'    | 1:A:211:A:C8      | 2.53        | 0.43     |
| 3:C:72:LYS:NZ    | 3:C:99:ASP:OD2    | 2.43        | 0.43     |
| 4:D:119:ARG:HD3  | 4:D:160:TYR:HB2   | 2.00        | 0.43     |
| 20:T:81:LYS:HB2  | 20:T:96:ILE:CG2   | 2.48        | 0.43     |
| 1:A:1497:U:H5''  | 1:A:1498:C:H5     | 1.83        | 0.43     |
| 1:A:2102:U:H2'   | 1:A:2103:C:C6     | 2.54        | 0.43     |
| 1:A:2293:C:H5''  | 14:N:89:ARG:HH12  | 1.84        | 0.43     |
| 1:A:2303:G:O2'   | 6:F:132:ASN:HB2   | 2.17        | 0.43     |
| 1:A:582:G:H2'    | 1:A:583:G:C8      | 2.53        | 0.43     |
| 4:D:36:ARG:HH21  | 4:D:88:GLY:HA2    | 1.84        | 0.43     |
| 10:J:106:LEU:HA  | 10:J:106:LEU:HD23 | 1.81        | 0.43     |
| 1:A:2406:U:N3    | 11:K:73:GLY:O     | 2.48        | 0.43     |
| 12:L:136:ALA:O   | 12:L:138:ASP:N    | 2.46        | 0.43     |
| 12:L:79:LEU:HA   | 12:L:79:LEU:HD22  | 1.82        | 0.43     |
| 19:S:67:GLY:O    | 19:S:69:TYR:N     | 2.43        | 0.43     |
| 23:W:49:VAL:HG11 | 23:W:70:VAL:HG11  | 1.98        | 0.43     |
| 1:A:2226:C:H2'   | 1:A:2227:A:O4'    | 2.18        | 0.43     |
| 1:A:2232:U:OP2   | 23:W:40:ARG:NH1   | 2.42        | 0.43     |
| 1:A:2306:C:H2'   | 1:A:2307:G:H21    | 1.83        | 0.43     |
| 1:A:270(F):U:H2' | 1:A:270(G):C:C6   | 2.53        | 0.43     |
| 3:C:145:VAL:HG11 | 3:C:175:LEU:HD11  | 2.00        | 0.43     |
| 8:H:124:GLY:O    | 8:H:142:VAL:HG23  | 2.18        | 0.43     |
| 20:T:97:ARG:HE   | 20:T:98:VAL:HB    | 1.83        | 0.43     |
| 1:A:476:G:H1'    | 1:A:480:A:N6      | 2.34        | 0.43     |
| 1:A:556:G:H8     | 1:A:556:G:O5'     | 2.00        | 0.43     |
| 1:A:974(A):C:H4' | 1:A:975:G:C5'     | 2.49        | 0.43     |
| 9:I:33:LEU:HA    | 9:I:38:HIS:CE1    | 2.54        | 0.43     |
| 9:I:58:ASP:HB3   | 9:I:95:PRO:HB3    | 2.00        | 0.43     |
| 14:N:29:PHE:HD1  | 14:N:92:TYR:HH    | 1.66        | 0.43     |
| 20:T:42:VAL:O    | 20:T:65:ALA:N     | 2.45        | 0.43     |
| 2:B:75:G:H4'     | 21:U:36:LYS:HG2   | 2.00        | 0.43     |
| 1:A:1337:G:H2'   | 1:A:1338:G:C8     | 2.53        | 0.43     |
| 1:A:134:C:H2'    | 1:A:135:G:H8      | 1.82        | 0.43     |
| 1:A:2713:A:OP1   | 13:M:14:SER:OG    | 2.30        | 0.43     |
| 12:L:116:GLU:O   | 12:L:120:ILE:HG12 | 2.17        | 0.43     |
| 15:O:1:MET:O     | 15:O:3:ARG:HG2    | 2.19        | 0.43     |
| 20:T:47:LYS:O    | 20:T:49:VAL:N     | 2.51        | 0.43     |
| 1:A:1638:C:H5''  | 1:A:2710:C:O2'    | 2.19        | 0.43     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:A:443:A:H1'     | 1:A:1201:C:O4'    | 2.17        | 0.43     |
| 11:K:90:ARG:HB3   | 11:K:91:PHE:H     | 1.68        | 0.43     |
| 1:A:1101:U:H2'    | 1:A:1102:C:H6     | 1.83        | 0.43     |
| 1:A:1291:C:H2'    | 1:A:1292:U:C6     | 2.52        | 0.43     |
| 1:A:1728:G:H5'    | 1:A:1729:A:OP2    | 2.18        | 0.43     |
| 1:A:1780:A:O2'    | 1:A:1781:C:O2     | 2.31        | 0.43     |
| 1:A:2170:A:H2'    | 1:A:2171:A:O4'    | 2.18        | 0.43     |
| 1:A:519:U:H2'     | 1:A:520:G:C8      | 2.54        | 0.43     |
| 4:D:179:GLU:HB3   | 4:D:181:LEU:HD22  | 1.99        | 0.43     |
| 4:D:14:ILE:H      | 4:D:21:VAL:HA     | 1.84        | 0.43     |
| 11:K:65:ARG:O     | 11:K:68:GLN:NE2   | 2.50        | 0.43     |
| 14:N:88:ASP:CG    | 14:N:89:ARG:H     | 2.21        | 0.43     |
| 18:R:20:VAL:HG22  | 18:R:47:VAL:HG21  | 2.00        | 0.43     |
| 20:T:55:TYR:CD1   | 20:T:55:TYR:N     | 2.87        | 0.43     |
| 20:T:46:LYS:HB2   | 20:T:61:ILE:HG22  | 1.99        | 0.43     |
| 1:A:1308:A:H2'    | 1:A:1309:G:O4'    | 2.17        | 0.43     |
| 1:A:2133:G:O2'    | 1:A:2158:A:N1     | 2.52        | 0.43     |
| 1:A:2376:A:H2'    | 1:A:2377:A:O4'    | 2.18        | 0.43     |
| 1:A:631:A:H2'     | 1:A:632:A:O4'     | 2.18        | 0.43     |
| 1:A:671:C:H2'     | 1:A:672:C:C6      | 2.54        | 0.43     |
| 3:C:35:LYS:HE3    | 3:C:64:ILE:C      | 2.39        | 0.43     |
| 5:E:9:ILE:HG23    | 5:E:20:LEU:O      | 2.18        | 0.43     |
| 11:K:18:ARG:HD2   | 11:K:27:HIS:CD2   | 2.54        | 0.43     |
| 12:L:20:ALA:HA    | 12:L:98:LYS:HB3   | 2.00        | 0.43     |
| 15:O:19:LEU:HA    | 15:O:20:PRO:HD3   | 1.86        | 0.43     |
| 1:A:1245:G:OP1    | 11:K:13:ASN:ND2   | 2.50        | 0.43     |
| 1:A:1444(A):A:H4' | 1:A:1460:A:O2'    | 2.18        | 0.43     |
| 1:A:1492:G:H3'    | 1:A:1493:C:H5'    | 2.01        | 0.43     |
| 1:A:2058:A:H8     | 1:A:2058:A:O5'    | 2.02        | 0.43     |
| 1:A:2336:A:H61    | 22:V:43:THR:CG2   | 2.32        | 0.43     |
| 1:A:2517:C:C2     | 1:A:2542:A:N6     | 2.87        | 0.43     |
| 1:A:2563:U:H2'    | 1:A:2565:A:OP2    | 2.19        | 0.43     |
| 1:A:2749:A:H4'    | 7:G:62:LYS:HB3    | 2.01        | 0.43     |
| 4:D:34:VAL:HG23   | 4:D:64:LYS:HZ2    | 1.84        | 0.43     |
| 8:H:68:LEU:HA     | 8:H:71:ILE:HG22   | 2.00        | 0.43     |
| 12:L:104:PHE:CE2  | 12:L:125:LEU:HD11 | 2.53        | 0.43     |
| 15:O:107:ASP:O    | 15:O:110:ILE:HG22 | 2.19        | 0.43     |
| 1:A:2059:A:H5'    | 1:A:2060:A:OP2    | 2.19        | 0.43     |
| 1:A:2684:U:OP1    | 15:O:53:ARG:HD3   | 2.19        | 0.43     |
| 1:A:2849:U:O4     | 15:O:23:ARG:NH2   | 2.40        | 0.43     |
| 1:A:395:U:H2'     | 1:A:396:G:C8      | 2.53        | 0.43     |
| 4:D:116:VAL:HG11  | 4:D:138:PRO:HB3   | 2.01        | 0.43     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 4:D:48:GLN:OE1    | 4:D:64:LYS:NZ     | 2.52        | 0.43     |
| 5:E:34:TRP:CE3    | 5:E:35:GLU:HG2    | 2.54        | 0.43     |
| 7:G:124:GLU:HB3   | 7:G:132:ARG:CG    | 2.48        | 0.43     |
| 8:H:31:LEU:HD11   | 8:H:38:LEU:HG     | 2.00        | 0.43     |
| 12:L:81:VAL:C     | 12:L:82:ARG:CG    | 2.85        | 0.43     |
| 14:N:12:PHE:HA    | 14:N:12:PHE:HD1   | 1.72        | 0.43     |
| 10:J:104:ARG:HD3  | 15:O:36:GLU:OE2   | 2.19        | 0.43     |
| 20:T:54:LYS:HB3   | 20:T:55:TYR:CD1   | 2.53        | 0.43     |
| 21:U:48:PHE:CE1   | 21:U:52:SER:HA    | 2.54        | 0.43     |
| 1:A:1022:G:H22    | 1:A:1142(A):A:H2  | 1.66        | 0.42     |
| 1:A:1543:A:HO2'   | 1:A:1544:C:H3'    | 1.82        | 0.42     |
| 1:A:2626:C:H2'    | 1:A:2627:G:O4'    | 2.19        | 0.42     |
| 1:A:2869:G:H2'    | 1:A:2870:C:O4'    | 2.18        | 0.42     |
| 3:C:169:GLU:N     | 3:C:172:TYR:O     | 2.52        | 0.42     |
| 4:D:117:MET:HB2   | 4:D:122:PHE:O     | 2.18        | 0.42     |
| 1:A:1005:C:O2'    | 9:I:28:THR:HG21   | 2.18        | 0.42     |
| 9:I:61:ARG:HE     | 9:I:61:ARG:HA     | 1.82        | 0.42     |
| 16:P:69:CYS:HB3   | 16:P:106:PHE:CZ   | 2.54        | 0.42     |
| 17:Q:64:HIS:CG    | 17:Q:92:THR:HG22  | 2.52        | 0.42     |
| 21:U:111:VAL:HG13 | 21:U:112:ARG:H    | 1.83        | 0.42     |
| 21:U:115:GLY:HA2  | 21:U:175:VAL:O    | 2.19        | 0.42     |
| 22:V:51:VAL:N     | 22:V:62:LEU:HD12  | 2.33        | 0.42     |
| 1:A:1126:A:OP1    | 1:A:1126:A:H8     | 2.03        | 0.42     |
| 1:A:1756:G:H4'    | 1:A:1758:G:O4'    | 2.19        | 0.42     |
| 1:A:2319:G:O6     | 14:N:4:LEU:HB2    | 2.19        | 0.42     |
| 1:A:2695:C:H2'    | 1:A:2696:U:H6     | 1.84        | 0.42     |
| 1:A:622:G:H2'     | 1:A:623:G:C8      | 2.54        | 0.42     |
| 4:D:22:PRO:HD2    | 4:D:22:PRO:O      | 2.19        | 0.42     |
| 7:G:153:LYS:HD2   | 7:G:153:LYS:N     | 2.33        | 0.42     |
| 9:I:89:LYS:O      | 9:I:93:THR:HG22   | 2.19        | 0.42     |
| 9:I:96:GLU:HB2    | 9:I:122:VAL:HG12  | 2.00        | 0.42     |
| 11:K:100:LEU:HA   | 11:K:100:LEU:HD22 | 1.77        | 0.42     |
| 1:A:994:C:OP1     | 16:P:53:ARG:NH2   | 2.52        | 0.42     |
| 21:U:69:THR:HG22  | 21:U:90:VAL:HA    | 1.99        | 0.42     |
| 1:A:1188:U:H4'    | 17:Q:79:VAL:HG22  | 2.00        | 0.42     |
| 1:A:1508:A:O2'    | 1:A:1509:C:O4'    | 2.36        | 0.42     |
| 1:A:177:G:H3'     | 1:A:178:G:C8      | 2.52        | 0.42     |
| 2:B:37:C:N3       | 2:B:48:A:O2'      | 2.47        | 0.42     |
| 3:C:123:ALA:HA    | 3:C:124:PRO:HD2   | 1.77        | 0.42     |
| 1:A:2679:A:H4'    | 4:D:165:VAL:HG11  | 2.01        | 0.42     |
| 8:H:52:ARG:CB     | 8:H:56:LYS:CB     | 2.88        | 0.42     |
| 8:H:88:ILE:HG12   | 8:H:88:ILE:H      | 1.65        | 0.42     |

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| Atom-1           | Atom-2            | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 13:M:113:LEU:HA  | 13:M:113:LEU:HD12 | 1.88        | 0.42     |
| 1:A:2820:A:C6    | 13:M:4:LEU:HD11   | 2.54        | 0.42     |
| 14:N:93:LYS:HB2  | 14:N:93:LYS:HE3   | 1.65        | 0.42     |
| 16:P:83:LEU:HD12 | 16:P:113:ALA:HB2  | 2.01        | 0.42     |
| 1:A:1184:G:OP1   | 25:Y:29:ARG:NH1   | 2.51        | 0.42     |
| 1:A:1543:A:H2    | 1:A:1545:A:C8     | 2.35        | 0.42     |
| 1:A:1819:A:H4'   | 1:A:1820:U:O5'    | 2.18        | 0.42     |
| 1:A:2119:A:C2    | 1:A:2171:A:H1'    | 2.55        | 0.42     |
| 1:A:2630:G:H2'   | 1:A:2631:G:C8     | 2.55        | 0.42     |
| 1:A:2633:G:H2'   | 1:A:2634:G:O4'    | 2.18        | 0.42     |
| 1:A:464:U:H2'    | 1:A:465:G:O4'     | 2.19        | 0.42     |
| 1:A:987:G:H2'    | 1:A:988:A:O4'     | 2.20        | 0.42     |
| 3:C:33:LEU:HB3   | 3:C:34:VAL:H      | 1.64        | 0.42     |
| 1:A:2723:C:OP2   | 4:D:109:LYS:NZ    | 2.52        | 0.42     |
| 4:D:9:VAL:HG23   | 4:D:26:ILE:HA     | 2.00        | 0.42     |
| 5:E:78:ILE:HG13  | 5:E:78:ILE:H      | 1.66        | 0.42     |
| 7:G:16:SER:OG    | 7:G:26:VAL:O      | 2.30        | 0.42     |
| 9:I:30:ILE:HG23  | 9:I:52:VAL:HG11   | 1.99        | 0.42     |
| 14:N:39:ILE:HD11 | 14:N:73:LEU:HD11  | 2.00        | 0.42     |
| 1:A:581:C:OP1    | 16:P:33:ARG:HG3   | 2.20        | 0.42     |
| 21:U:181:GLU:HB3 | 21:U:182:LYS:H    | 1.61        | 0.42     |
| 1:A:139:G:N2     | 1:A:141:A:N1      | 2.64        | 0.42     |
| 1:A:1470:G:N2    | 1:A:1522:G:OP2    | 2.52        | 0.42     |
| 1:A:1641:A:H2'   | 1:A:1642:G:O4'    | 2.20        | 0.42     |
| 1:A:1860:G:H2'   | 1:A:1861:G:H8     | 1.84        | 0.42     |
| 1:A:2282:G:H4'   | 1:A:2389:G:O2'    | 2.20        | 0.42     |
| 1:A:323:G:H2'    | 5:E:169:ASN:ND2   | 2.35        | 0.42     |
| 1:A:323:G:C2     | 1:A:333:G:H1'     | 2.54        | 0.42     |
| 1:A:884:C:N3     | 1:A:892:G:C6      | 2.87        | 0.42     |
| 6:F:97:ASP:HA    | 6:F:100:TRP:HD1   | 1.85        | 0.42     |
| 6:F:159:VAL:HG21 | 6:F:173:LEU:HD11  | 2.00        | 0.42     |
| 7:G:6:ARG:HG3    | 7:G:7:LEU:HG      | 2.01        | 0.42     |
| 15:O:26:ASP:HB3  | 15:O:92:GLY:N     | 2.18        | 0.42     |
| 16:P:75:ASN:HB2  | 16:P:78:THR:H     | 1.85        | 0.42     |
| 20:T:50:ARG:HG2  | 20:T:50:ARG:H     | 1.67        | 0.42     |
| 21:U:169:GLU:O   | 21:U:171:ILE:HG23 | 2.19        | 0.42     |
| 1:A:1016:G:H2'   | 1:A:1017:G:O4'    | 2.19        | 0.42     |
| 1:A:1794:U:H2'   | 1:A:1795:C:H6     | 1.83        | 0.42     |
| 1:A:579:G:O2'    | 1:A:2019:A:OP1    | 2.29        | 0.42     |
| 1:A:2422:A:H2'   | 1:A:2424:C:C6     | 2.55        | 0.42     |
| 1:A:2517:C:O3'   | 1:A:2518:A:H3'    | 2.19        | 0.42     |
| 1:A:247:G:H4'    | 1:A:386:G:C4      | 2.54        | 0.42     |

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| Atom-1           | Atom-2            | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 1:A:456:C:O2'    | 1:A:457:A:H5'     | 2.19        | 0.42     |
| 1:A:918:A:N3     | 2:B:80:U:O2'      | 2.41        | 0.42     |
| 6:F:173:LEU:O    | 6:F:178:PHE:HB2   | 2.20        | 0.42     |
| 13:M:63:ARG:HA   | 13:M:80:PHE:CZ    | 2.54        | 0.42     |
| 19:S:44:GLU:O    | 19:S:48:LYS:N     | 2.52        | 0.42     |
| 21:U:103:ARG:HD3 | 21:U:136:PHE:CG   | 2.54        | 0.42     |
| 1:A:184:C:H2'    | 1:A:185:U:C6      | 2.55        | 0.42     |
| 1:A:2437:U:H2'   | 1:A:2438:U:C6     | 2.55        | 0.42     |
| 1:A:2729:G:H1'   | 4:D:187:ALA:HB2   | 2.01        | 0.42     |
| 2:B:52:A:O2'     | 2:B:53:A:N7       | 2.51        | 0.42     |
| 2:B:5:C:OP1      | 2:B:61:G:O2'      | 2.33        | 0.42     |
| 3:C:96:HIS:NE2   | 3:C:102:LYS:HE2   | 2.34        | 0.42     |
| 1:A:1803:A:H4'   | 3:C:259:THR:HG23  | 2.01        | 0.42     |
| 4:D:78:LEU:HG    | 4:D:79:ARG:NE     | 2.35        | 0.42     |
| 5:E:182:ASN:O    | 5:E:186:ILE:HG12  | 2.20        | 0.42     |
| 6:F:151:ALA:HB3  | 6:F:153:ARG:NH1   | 2.35        | 0.42     |
| 9:I:35:ARG:HB2   | 9:I:42:TRP:CZ3    | 2.55        | 0.42     |
| 24:X:70:GLN:O    | 24:X:71:ASN:HB2   | 2.19        | 0.42     |
| 26:Z:14:ILE:HG22 | 26:Z:24:THR:HG22  | 2.01        | 0.42     |
| 1:A:1051:G:H2'   | 1:A:1052:C:O4'    | 2.19        | 0.42     |
| 1:A:1479:G:H2'   | 1:A:1480:G:O4'    | 2.20        | 0.42     |
| 1:A:1991:U:H2'   | 1:A:1992:G:H5''   | 2.01        | 0.42     |
| 1:A:2391:G:C6    | 1:A:2427:C:H1'    | 2.55        | 0.42     |
| 1:A:2392:A:H2    | 1:A:2424:C:H42    | 1.65        | 0.42     |
| 1:A:590:A:H2'    | 1:A:591:C:C6      | 2.55        | 0.42     |
| 2:B:17:C:H2'     | 2:B:18:G:O4'      | 2.19        | 0.42     |
| 3:C:245:PRO:HA   | 3:C:246:PRO:HD3   | 1.95        | 0.42     |
| 4:D:21:VAL:HG23  | 4:D:22:PRO:CG     | 2.41        | 0.42     |
| 5:E:28:ILE:HG13  | 5:E:28:ILE:H      | 1.68        | 0.42     |
| 7:G:105:LEU:HD22 | 7:G:113:VAL:HB    | 2.01        | 0.42     |
| 7:G:164:TYR:O    | 7:G:166:GLY:N     | 2.52        | 0.42     |
| 14:N:14:VAL:HG11 | 14:N:90:GLY:O     | 2.19        | 0.42     |
| 18:R:75:TYR:CZ   | 18:R:104:THR:HG21 | 2.55        | 0.42     |
| 23:W:90:ILE:O    | 23:W:94:LEU:HB2   | 2.20        | 0.42     |
| 1:A:1268:A:OP1   | 1:A:2006:C:OP1    | 2.37        | 0.42     |
| 1:A:1321:A:H2'   | 1:A:1322:A:O4'    | 2.19        | 0.42     |
| 1:A:2215:G:H2'   | 1:A:2216:G:H8     | 1.85        | 0.42     |
| 1:A:921:G:H4'    | 1:A:2269:A:C5     | 2.55        | 0.42     |
| 1:A:2415:G:H5'   | 11:K:67:MET:H     | 1.85        | 0.42     |
| 3:C:35:LYS:HB3   | 3:C:36:PRO:HA     | 2.01        | 0.42     |
| 5:E:184:TYR:O    | 5:E:188:ARG:HG3   | 2.19        | 0.42     |
| 6:F:116:ASP:OD1  | 6:F:116:ASP:N     | 2.53        | 0.42     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 6:F:47:LYS:HD3   | 6:F:81:LYS:CB    | 2.49        | 0.42     |
| 7:G:4:ILE:HB     | 7:G:6:ARG:HG2    | 2.01        | 0.42     |
| 12:L:18:LYS:HB3  | 12:L:19:GLY:H    | 1.50        | 0.42     |
| 14:N:78:LEU:HA   | 14:N:78:LEU:HD23 | 1.86        | 0.42     |
| 21:U:94:GLU:HB2  | 21:U:130:PRO:HD2 | 2.02        | 0.42     |
| 25:Y:35:ARG:HB3  | 25:Y:37:LEU:HD21 | 2.01        | 0.42     |
| 1:A:2143:C:H2'   | 1:A:2144:U:O4'   | 2.20        | 0.42     |
| 1:A:2246:G:H2'   | 1:A:2247:A:C8    | 2.55        | 0.42     |
| 1:A:242:G:H1'    | 1:A:243:U:OP2    | 2.20        | 0.42     |
| 1:A:2469:A:H4'   | 1:A:2469:A:OP1   | 2.20        | 0.42     |
| 1:A:2704:C:H2'   | 1:A:2705:A:O4'   | 2.19        | 0.42     |
| 1:A:675:A:N3     | 1:A:2443:C:O2'   | 2.45        | 0.42     |
| 1:A:833:U:H2'    | 1:A:834:C:C6     | 2.55        | 0.42     |
| 2:B:14:U:H4'     | 2:B:70:C:O2      | 2.20        | 0.42     |
| 4:D:13:ARG:HB3   | 11:K:63:PRO:HA   | 125.34      | 0.42     |
| 7:G:10:PRO:HD2   | 7:G:50:VAL:O     | 2.20        | 0.42     |
| 15:O:51:ARG:HG3  | 15:O:98:LYS:HG3  | 2.02        | 0.42     |
| 16:P:58:ARG:NH1  | 16:P:93:LYS:HE2  | 2.35        | 0.42     |
| 23:W:85:LEU:HA   | 23:W:87:PRO:HD2  | 2.01        | 0.42     |
| 6:F:6:ALA:N      | 26:Z:23:GLU:HG2  | 2.31        | 0.42     |
| 1:A:1510:A:N3    | 1:A:1510:A:H2'   | 2.35        | 0.41     |
| 1:A:2245:U:H5'   | 1:A:2246:G:H5'   | 2.02        | 0.41     |
| 1:A:2286:A:H4'   | 1:A:2287:A:O4'   | 2.19        | 0.41     |
| 1:A:2313:C:H5''  | 6:F:91:ARG:HD3   | 2.01        | 0.41     |
| 1:A:2405:G:H1'   | 1:A:2412:A:N6    | 2.35        | 0.41     |
| 1:A:2461:C:H2'   | 1:A:2462:U:C6    | 2.54        | 0.41     |
| 1:A:2699:C:H2'   | 1:A:2700:C:O4'   | 2.20        | 0.41     |
| 1:A:611:C:H2'    | 1:A:612:G:C8     | 2.55        | 0.41     |
| 1:A:784:A:O4'    | 3:C:227:ASN:ND2  | 2.53        | 0.41     |
| 3:C:101:GLU:OE1  | 3:C:103:ARG:NH1  | 2.53        | 0.41     |
| 3:C:61:LEU:HD12  | 3:C:61:LEU:HA    | 1.77        | 0.41     |
| 4:D:188:VAL:HG23 | 4:D:189:PRO:HD2  | 2.01        | 0.41     |
| 5:E:129:PHE:O    | 5:E:130:ALA:HB3  | 2.20        | 0.41     |
| 5:E:93:LYS:HB3   | 5:E:94:PRO:HD2   | 2.01        | 0.41     |
| 7:G:125:VAL:HG13 | 7:G:126:PRO:HG3  | 2.01        | 0.41     |
| 10:J:7:TYR:CE1   | 10:J:20:MET:HB2  | 2.55        | 0.41     |
| 25:Y:7:LYS:HA    | 25:Y:33:GLN:O    | 2.20        | 0.41     |
| 26:Z:55:ARG:O    | 26:Z:59:PHE:HB3  | 2.20        | 0.41     |
| 1:A:1694:C:H4'   | 1:A:1695:G:O5'   | 2.19        | 0.41     |
| 2:B:7:G:H5'      | 14:N:29:PHE:CE2  | 2.55        | 0.41     |
| 3:C:43:ARG:HB2   | 3:C:54:ARG:HB2   | 2.02        | 0.41     |
| 4:D:76:ARG:HD2   | 4:D:76:ARG:N     | 2.35        | 0.41     |

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| Atom-1           | Atom-2            | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 5:E:46:ARG:HH11  | 5:E:46:ARG:HG2    | 1.84        | 0.41     |
| 1:A:2305:A:O5'   | 6:F:134:GLY:HA3   | 2.19        | 0.41     |
| 8:H:135:GLU:HB2  | 8:H:136:VAL:H     | 1.77        | 0.41     |
| 9:I:10:GLU:HA    | 9:I:11:PRO:HD3    | 1.65        | 0.41     |
| 12:L:17:LEU:HD21 | 12:L:41:TRP:HD1   | 1.84        | 0.41     |
| 12:L:68:ILE:HD13 | 12:L:103:MET:HG2  | 2.02        | 0.41     |
| 22:V:23:VAL:HA   | 22:V:38:VAL:HG22  | 2.00        | 0.41     |
| 1:A:1366:A:H2'   | 1:A:1367:A:O4'    | 2.19        | 0.41     |
| 1:A:1506:C:H3'   | 1:A:1507:A:H5''   | 2.02        | 0.41     |
| 1:A:1543:A:N3    | 1:A:1545:A:N9     | 2.68        | 0.41     |
| 5:E:177:ALA:HB1  | 5:E:178:PRO:HD2   | 2.03        | 0.41     |
| 11:K:20:GLY:HA2  | 11:K:27:HIS:O     | 2.19        | 0.41     |
| 11:K:81:GLN:HG2  | 11:K:106:LEU:HD23 | 2.02        | 0.41     |
| 13:M:109:ALA:HA  | 13:M:110:PRO:HD2  | 1.95        | 0.41     |
| 13:M:22:ARG:HA   | 13:M:47:PHE:HE2   | 1.86        | 0.41     |
| 14:N:108:GLY:O   | 14:N:110:LEU:HG   | 2.20        | 0.41     |
| 17:Q:76:LYS:HB2  | 17:Q:81:TYR:HB3   | 2.01        | 0.41     |
| 21:U:110:GLY:HA2 | 21:U:111:VAL:O    | 2.19        | 0.41     |
| 1:A:1259:G:H2'   | 1:A:1260:G:C8     | 2.55        | 0.41     |
| 1:A:2298:A:H2'   | 1:A:2299:G:O4'    | 2.21        | 0.41     |
| 1:A:2702:U:H2'   | 1:A:2702:U:O2     | 2.20        | 0.41     |
| 1:A:669:G:H2'    | 1:A:669:G:N3      | 2.36        | 0.41     |
| 1:A:464:U:C2     | 1:A:788:A:C6      | 3.09        | 0.41     |
| 1:A:839:U:H1'    | 1:A:1191:G:H1'    | 2.02        | 0.41     |
| 1:A:847:U:O4     | 1:A:933:A:C6      | 2.70        | 0.41     |
| 5:E:164:ARG:HG3  | 5:E:175:THR:OG1   | 2.20        | 0.41     |
| 5:E:113:ALA:HB1  | 5:E:186:ILE:HG21  | 2.02        | 0.41     |
| 6:F:6:ALA:HB3    | 6:F:104:GLU:OE2   | 2.20        | 0.41     |
| 12:L:58:PHE:HD1  | 12:L:61:GLY:HA3   | 1.85        | 0.41     |
| 14:N:14:VAL:HG21 | 14:N:89:ARG:HG2   | 2.02        | 0.41     |
| 20:T:88:LYS:HA   | 20:T:88:LYS:NZ    | 2.35        | 0.41     |
| 1:A:1130:U:O2'   | 1:A:1131:G:P      | 2.79        | 0.41     |
| 1:A:1204:A:H1'   | 1:A:1206:G:C4     | 2.55        | 0.41     |
| 1:A:1297:C:H2'   | 1:A:1298:C:H6     | 1.85        | 0.41     |
| 1:A:1812:A:H2'   | 1:A:1813:G:H8     | 1.84        | 0.41     |
| 1:A:2150:U:H2'   | 1:A:2151:G:H8     | 1.84        | 0.41     |
| 1:A:2554:U:H2'   | 1:A:2555:U:C6     | 2.55        | 0.41     |
| 1:A:2665:A:H2'   | 1:A:2666:C:O4'    | 2.21        | 0.41     |
| 1:A:2712:U:O2'   | 1:A:2712(A):A:C8  | 2.72        | 0.41     |
| 1:A:27:G:HO2'    | 1:A:28:A:P        | 2.42        | 0.41     |
| 1:A:592:G:H1     | 1:A:665:C:H42     | 1.68        | 0.41     |
| 3:C:257:LEU:HD23 | 3:C:257:LEU:HA    | 1.90        | 0.41     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 3:C:35:LYS:HE3   | 3:C:63:ARG:C     | 2.41        | 0.41     |
| 5:E:178:PRO:HB2  | 5:E:201:VAL:CG1  | 2.51        | 0.41     |
| 6:F:124:SER:HB2  | 6:F:131:TYR:CE1  | 2.56        | 0.41     |
| 6:F:27:ASN:HB3   | 6:F:30:GLU:HG3   | 2.01        | 0.41     |
| 6:F:98:ARG:HE    | 6:F:98:ARG:HB2   | 1.38        | 0.41     |
| 1:A:2415:G:C5'   | 11:K:67:MET:H    | 2.34        | 0.41     |
| 12:L:40:ALA:O    | 12:L:42:ILE:HD12 | 2.21        | 0.41     |
| 19:S:40:LYS:C    | 19:S:42:ALA:H    | 2.23        | 0.41     |
| 20:T:84:ARG:HD3  | 20:T:86:ARG:NH1  | 2.35        | 0.41     |
| 21:U:99:TYR:HB3  | 21:U:123:ASP:HB2 | 2.03        | 0.41     |
| 1:A:1190:G:OP1   | 11:K:30:THR:OG1  | 2.20        | 0.41     |
| 1:A:1636:C:H2'   | 1:A:1637:A:H8    | 1.82        | 0.41     |
| 1:A:1921:G:H2'   | 1:A:1922:G:H8    | 1.86        | 0.41     |
| 1:A:512:G:H1'    | 1:A:513:A:OP2    | 2.18        | 0.41     |
| 1:A:705:A:H2'    | 1:A:706:A:O4'    | 2.20        | 0.41     |
| 1:A:820:A:H1'    | 1:A:943:U:H1'    | 2.02        | 0.41     |
| 5:E:29:ASN:O     | 5:E:112:MET:HE1  | 2.21        | 0.41     |
| 9:I:47:ALA:HB2   | 9:I:112:LEU:HD11 | 2.02        | 0.41     |
| 19:S:51:VAL:HG13 | 19:S:81:VAL:HG23 | 2.03        | 0.41     |
| 20:T:54:LYS:HB3  | 20:T:55:TYR:CE1  | 2.55        | 0.41     |
| 1:A:1259:G:H2'   | 1:A:1260:G:H8    | 1.86        | 0.41     |
| 1:A:945:A:C4     | 1:A:2448:A:C2    | 3.08        | 0.41     |
| 1:A:709:U:H2'    | 1:A:710:G:H8     | 1.86        | 0.41     |
| 1:A:868:U:H2'    | 1:A:869:G:O4'    | 2.20        | 0.41     |
| 1:A:947:G:H2'    | 1:A:948:G:H8     | 1.85        | 0.41     |
| 4:D:92:THR:HB    | 4:D:93:VAL:H     | 1.55        | 0.41     |
| 6:F:47:LYS:HE3   | 6:F:47:LYS:HB2   | 1.81        | 0.41     |
| 13:M:10:LEU:O    | 13:M:12:ARG:HG3  | 2.21        | 0.41     |
| 16:P:61:TRP:O    | 16:P:65:ILE:HG13 | 2.21        | 0.41     |
| 1:A:48:G:H22     | 1:A:177:G:H5''   | 1.84        | 0.41     |
| 1:A:210:C:H4'    | 1:A:1367:A:H1'   | 2.02        | 0.41     |
| 1:A:588:U:H1'    | 5:E:90:PHE:CG    | 2.56        | 0.41     |
| 1:A:848:G:O6     | 1:A:929:G:H2'    | 2.21        | 0.41     |
| 1:A:862:G:H2'    | 1:A:863:A:O4'    | 2.21        | 0.41     |
| 1:A:859:G:N2     | 1:A:917:A:OP2    | 2.49        | 0.41     |
| 3:C:127:VAL:HA   | 3:C:193:VAL:HG22 | 2.02        | 0.41     |
| 1:A:782:A:O2'    | 3:C:225:ALA:HB1  | 2.20        | 0.41     |
| 4:D:20:ALA:O     | 4:D:21:VAL:CG1   | 2.51        | 0.41     |
| 4:D:35:GLN:HB3   | 4:D:48:GLN:HB2   | 2.02        | 0.41     |
| 7:G:33:LEU:HD11  | 7:G:136:ILE:O    | 2.20        | 0.41     |
| 7:G:4:ILE:O      | 7:G:6:ARG:N      | 2.51        | 0.41     |
| 8:H:14:ASP:O     | 8:H:16:GLY:N     | 2.54        | 0.41     |

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| Atom-1           | Atom-2            | Distance(Å) | Clash(Å) |
|------------------|-------------------|-------------|----------|
| 9:I:57:ALA:C     | 9:I:60:ILE:HD11   | 2.40        | 0.41     |
| 9:I:57:ALA:O     | 9:I:60:ILE:HD11   | 2.21        | 0.41     |
| 9:I:71:ILE:HG21  | 9:I:84:LYS:HB3    | 2.02        | 0.41     |
| 15:O:91:ARG:HB2  | 15:O:121:ILE:HG13 | 2.03        | 0.41     |
| 1:A:1070:A:N7    | 1:A:1096:A:H2'    | 2.36        | 0.41     |
| 1:A:1091:G:N2    | 1:A:1101:U:H1'    | 2.36        | 0.41     |
| 1:A:2414:G:H21   | 11:K:67:MET:CE    | 2.33        | 0.41     |
| 1:A:2820:A:O2'   | 1:A:2821:A:OP1    | 2.34        | 0.41     |
| 2:B:13:A:H2'     | 2:B:14:U:H5''     | 2.02        | 0.41     |
| 1:A:797:C:OP2    | 5:E:62:ARG:HB2    | 2.21        | 0.41     |
| 7:G:125:VAL:HG13 | 7:G:126:PRO:CG    | 2.46        | 0.41     |
| 7:G:152:ARG:HE   | 7:G:153:LYS:HZ3   | 1.69        | 0.41     |
| 8:H:12:LEU:HG    | 8:H:19:VAL:HG11   | 2.03        | 0.41     |
| 10:J:26:LYS:HB2  | 10:J:30:ALA:HB2   | 2.02        | 0.41     |
| 10:J:73:ASP:OD2  | 15:O:32:TYR:OH    | 2.28        | 0.41     |
| 1:A:566:U:OP1    | 11:K:29:LYS:HE2   | 2.21        | 0.41     |
| 22:V:12:ASN:HB3  | 22:V:13:GLY:H     | 1.67        | 0.41     |
| 23:W:58:ILE:CD1  | 23:W:86:SER:HB2   | 2.50        | 0.41     |
| 26:Z:39:CYS:HB2  | 26:Z:41:PRO:HD2   | 2.02        | 0.41     |
| 1:A:1752:C:H42   | 1:A:1756:G:H1     | 1.69        | 0.41     |
| 1:A:217:G:H2'    | 1:A:218:A:O4'     | 2.21        | 0.41     |
| 1:A:2697:G:H2'   | 1:A:2698:U:O4'    | 2.21        | 0.41     |
| 1:A:328:U:H4'    | 20:T:68:HIS:CD2   | 2.56        | 0.41     |
| 1:A:755:C:H2'    | 1:A:756:C:C6      | 2.56        | 0.41     |
| 1:A:840:C:H2'    | 1:A:841:A:C8      | 2.56        | 0.41     |
| 2:B:79:C:H2'     | 2:B:80:U:O4'      | 2.20        | 0.41     |
| 3:C:111:LEU:HD23 | 3:C:111:LEU:HA    | 1.78        | 0.41     |
| 3:C:150:LYS:HD3  | 3:C:150:LYS:N     | 2.36        | 0.41     |
| 3:C:226:MET:HB3  | 3:C:230:ASP:HB2   | 2.03        | 0.41     |
| 3:C:34:VAL:C     | 3:C:35:LYS:HG3    | 2.40        | 0.41     |
| 4:D:144:ARG:HB3  | 4:D:145:LYS:H     | 1.47        | 0.41     |
| 9:I:73:THR:HB    | 9:I:82:LEU:HD11   | 2.02        | 0.41     |
| 9:I:9:VAL:HG21   | 9:I:48:MET:HB3    | 2.02        | 0.41     |
| 11:K:62:LEU:N    | 11:K:62:LEU:HD13  | 2.36        | 0.41     |
| 12:L:66:ILE:HG13 | 12:L:67:ARG:N     | 2.36        | 0.41     |
| 14:N:62:LYS:HB3  | 14:N:97:ARG:CD    | 2.44        | 0.41     |
| 21:U:74:VAL:HG22 | 21:U:86:VAL:HG22  | 2.03        | 0.41     |
| 21:U:97:GLU:O    | 21:U:98:MET:HB3   | 2.21        | 0.41     |
| 1:A:1179:C:H2'   | 1:A:1180:C:O4'    | 2.20        | 0.41     |
| 1:A:2168:G:H8    | 1:A:2168:G:OP2    | 2.04        | 0.41     |
| 1:A:242:G:H4'    | 1:A:243:U:O5'     | 2.21        | 0.41     |
| 1:A:2692:C:H2'   | 1:A:2693:A:C8     | 2.55        | 0.41     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:A:700:G:H2'     | 1:A:701:G:O4'     | 2.21        | 0.41     |
| 5:E:33:LEU:HA     | 5:E:33:LEU:HD12   | 1.83        | 0.41     |
| 6:F:131:TYR:O     | 6:F:159:VAL:HG13  | 2.21        | 0.41     |
| 7:G:107:VAL:HB    | 7:G:153:LYS:HE3   | 2.03        | 0.41     |
| 8:H:120:ILE:HD11  | 8:H:126:TYR:OH    | 2.20        | 0.41     |
| 13:M:70:LEU:C     | 13:M:72:ASP:H     | 2.21        | 0.41     |
| 14:N:83:LYS:C     | 14:N:109:GLY:HA3  | 2.42        | 0.41     |
| 16:P:83:LEU:HG    | 16:P:88:ILE:HB    | 2.03        | 0.41     |
| 19:S:67:GLY:C     | 19:S:69:TYR:H     | 2.23        | 0.41     |
| 21:U:110:GLY:CA   | 21:U:111:VAL:C    | 2.87        | 0.41     |
| 26:Z:23:GLU:HG3   | 26:Z:25:TYR:HE2   | 1.85        | 0.41     |
| 1:A:1024:G:C6     | 1:A:1025:G:C6     | 3.09        | 0.40     |
| 1:A:1676:A:H2'    | 1:A:1677:A:O4'    | 2.21        | 0.40     |
| 1:A:2315:G:H2'    | 1:A:2316:C:C6     | 2.56        | 0.40     |
| 1:A:2322:A:H2'    | 1:A:2323:G:O4'    | 2.21        | 0.40     |
| 1:A:2845:G:O2'    | 1:A:2846:G:H5'    | 2.21        | 0.40     |
| 1:A:2032:G:H1'    | 4:D:145:LYS:HD3   | 2.03        | 0.40     |
| 4:D:184:VAL:HB    | 4:D:185:LYS:H     | 1.64        | 0.40     |
| 5:E:107:LYS:HE3   | 5:E:206:ILE:HD12  | 2.03        | 0.40     |
| 6:F:117:PHE:HE1   | 6:F:120:LEU:HD23  | 1.86        | 0.40     |
| 10:J:63:VAL:HB    | 10:J:106:LEU:HD11 | 2.02        | 0.40     |
| 15:O:109:GLU:O    | 15:O:113:LYS:HB2  | 2.21        | 0.40     |
| 15:O:51:ARG:CG    | 15:O:98:LYS:HG3   | 2.51        | 0.40     |
| 22:V:72:ARG:HB2   | 22:V:75:LEU:HB2   | 2.03        | 0.40     |
| 26:Z:13:ARG:O     | 26:Z:30:GLU:HA    | 2.21        | 0.40     |
| 4:D:197:ILE:HD11  | 4:D:199:ARG:CZ    | 2.50        | 0.40     |
| 4:D:55:ASN:HD22   | 4:D:58:ARG:HB2    | 1.87        | 0.40     |
| 7:G:98:LEU:HB2    | 7:G:125:VAL:HB    | 2.03        | 0.40     |
| 8:H:30:LEU:HD22   | 8:H:35:LEU:HD11   | 2.02        | 0.40     |
| 11:K:114:ILE:HD11 | 11:K:130:PHE:CD2  | 2.57        | 0.40     |
| 12:L:58:PHE:CD1   | 12:L:61:GLY:HA3   | 2.56        | 0.40     |
| 1:A:1649:G:O2'    | 13:M:107:ASP:OD2  | 2.32        | 0.40     |
| 1:A:2685:G:P      | 15:O:51:ARG:HH22  | 2.44        | 0.40     |
| 1:A:1614:A:H62    | 18:R:93:ALA:HB2   | 1.85        | 0.40     |
| 21:U:48:PHE:HE1   | 21:U:71:VAL:HG21  | 1.87        | 0.40     |
| 1:A:1430:C:H2'    | 1:A:1431:U:C6     | 2.57        | 0.40     |
| 1:A:2262:U:H2'    | 1:A:2263:C:C6     | 2.56        | 0.40     |
| 1:A:303:U:H2'     | 1:A:304:G:C8      | 2.56        | 0.40     |
| 1:A:341:G:H2'     | 1:A:342:G:O4'     | 2.21        | 0.40     |
| 1:A:722:A:H3'     | 1:A:723:G:H8      | 1.87        | 0.40     |
| 1:A:960:A:H5''    | 1:A:961:C:OP1     | 2.22        | 0.40     |
| 3:C:26:LYS:HD2    | 3:C:26:LYS:H      | 1.87        | 0.40     |

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| Atom-1           | Atom-2           | Distance(Å) | Clash(Å) |
|------------------|------------------|-------------|----------|
| 4:D:13:ARG:HB2   | 11:K:62:LEU:O    | 125.80      | 0.40     |
| 7:G:103:LEU:HG   | 7:G:105:LEU:HD12 | 2.02        | 0.40     |
| 14:N:23:ARG:HB2  | 14:N:86:ALA:HB2  | 2.03        | 0.40     |
| 21:U:92:SER:HB3  | 21:U:93:ASP:H    | 1.66        | 0.40     |
| 1:A:1011:G:C2    | 1:A:1013:C:C2    | 3.10        | 0.40     |
| 1:A:1061:U:H3'   | 1:A:1062:G:H5''  | 2.02        | 0.40     |
| 1:A:1174:A:H2'   | 1:A:1174:A:N3    | 2.35        | 0.40     |
| 1:A:121:G:H4'    | 1:A:149:A:H5'    | 2.03        | 0.40     |
| 1:A:1312:U:H1'   | 1:A:1313:U:OP2   | 2.22        | 0.40     |
| 1:A:2605:U:H2'   | 1:A:2606:C:C6    | 2.56        | 0.40     |
| 1:A:631:A:N3     | 1:A:2415:G:O2'   | 2.47        | 0.40     |
| 2:B:38:C:O2      | 2:B:48:A:H1'     | 2.22        | 0.40     |
| 3:C:96:HIS:CD2   | 3:C:102:LYS:HG2  | 2.56        | 0.40     |
| 3:C:35:LYS:HB3   | 3:C:63:ARG:HA    | 2.04        | 0.40     |
| 4:D:26:ILE:O     | 4:D:26:ILE:HG12  | 2.18        | 0.40     |
| 4:D:36:ARG:HH11  | 4:D:36:ARG:HB3   | 1.87        | 0.40     |
| 5:E:116:ASP:OD2  | 11:K:1:MET:N     | 2.54        | 0.40     |
| 5:E:181:LEU:HA   | 5:E:181:LEU:HD22 | 1.79        | 0.40     |
| 5:E:29:ASN:HB3   | 5:E:32:LEU:HD23  | 2.04        | 0.40     |
| 7:G:30:LYS:HD2   | 7:G:81:GLU:H     | 1.86        | 0.40     |
| 8:H:138:ILE:HG12 | 8:H:139:GLN:N    | 2.37        | 0.40     |
| 9:I:108:PRO:O    | 9:I:113:GLY:HA3  | 2.21        | 0.40     |
| 12:L:72:LYS:HB3  | 12:L:94:VAL:O    | 2.22        | 0.40     |
| 15:O:120:ARG:HA  | 15:O:123:GLN:NE2 | 2.37        | 0.40     |
| 20:T:11:ASP:O    | 20:T:26:LYS:HG3  | 2.21        | 0.40     |
| 20:T:64:GLU:HG2  | 20:T:64:GLU:H    | 1.64        | 0.40     |
| 23:W:87:PRO:O    | 23:W:91:LYS:HB2  | 2.21        | 0.40     |
| 23:W:95:LEU:HA   | 23:W:95:LEU:HD23 | 1.94        | 0.40     |
| 1:A:2123:G:H2'   | 1:A:2124:G:C8    | 2.54        | 0.40     |
| 1:A:2308:G:C2    | 1:A:2311:A:H2    | 2.37        | 0.40     |
| 1:A:380:U:H2'    | 1:A:381:G:C8     | 2.56        | 0.40     |
| 1:A:71:A:H5''    | 1:A:72:U:O5'     | 2.21        | 0.40     |
| 1:A:196:A:O2'    | 1:A:805:G:O6     | 2.32        | 0.40     |
| 1:A:955:C:OP2    | 12:L:14:ARG:HD2  | 2.21        | 0.40     |
| 3:C:209:ALA:O    | 3:C:212:SER:HB2  | 2.22        | 0.40     |
| 3:C:44:ASN:HB2   | 3:C:49:ILE:HA    | 2.02        | 0.40     |
| 9:I:17:ASP:O     | 9:I:19:GLU:N     | 2.54        | 0.40     |
| 10:J:66:LYS:HA   | 10:J:79:PHE:O    | 2.22        | 0.40     |
| 11:K:25:SER:OG   | 11:K:26:GLY:O    | 2.38        | 0.40     |
| 15:O:26:ASP:CB   | 15:O:91:ARG:HA   | 2.52        | 0.40     |
| 16:P:66:ASN:CG   | 16:P:70:ARG:HH21 | 2.21        | 0.40     |
| 21:U:10:ARG:HH21 | 21:U:26:GLY:H    | 1.69        | 0.40     |

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| Atom-1          | Atom-2          | Distance(Å) | Clash(Å) |
|-----------------|-----------------|-------------|----------|
| 22:V:68:GLU:HG2 | 22:V:80:HIS:HB2 | 2.04        | 0.40     |
| 1:A:379:G:N2    | 23:W:42:GLN:OE1 | 2.48        | 0.40     |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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 |    |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 3   | C     | 270/276 (98%) | 226 (84%) | 32 (12%) | 12 (4%)  | 4           | 45 |
| 4   | D     | 203/206 (98%) | 148 (73%) | 35 (17%) | 20 (10%) | 1           | 18 |
| 5   | E     | 200/210 (95%) | 170 (85%) | 18 (9%)  | 12 (6%)  | 2           | 34 |
| 6   | F     | 179/182 (98%) | 139 (78%) | 26 (14%) | 14 (8%)  | 1           | 25 |
| 7   | G     | 168/180 (93%) | 116 (69%) | 33 (20%) | 19 (11%) | 1           | 14 |
| 8   | H     | 144/148 (97%) | 104 (72%) | 27 (19%) | 13 (9%)  | 1           | 21 |
| 9   | I     | 136/140 (97%) | 104 (76%) | 20 (15%) | 12 (9%)  | 1           | 22 |
| 10  | J     | 120/122 (98%) | 109 (91%) | 9 (8%)   | 2 (2%)   | 14          | 70 |
| 11  | K     | 148/150 (99%) | 106 (72%) | 28 (19%) | 14 (10%) | 1           | 19 |
| 12  | L     | 139/141 (99%) | 99 (71%)  | 22 (16%) | 18 (13%) | 0           | 11 |
| 13  | M     | 116/118 (98%) | 106 (91%) | 5 (4%)   | 5 (4%)   | 4           | 46 |
| 14  | N     | 109/112 (97%) | 76 (70%)  | 22 (20%) | 11 (10%) | 1           | 17 |
| 15  | O     | 135/146 (92%) | 107 (79%) | 16 (12%) | 12 (9%)  | 1           | 21 |
| 16  | P     | 115/118 (98%) | 102 (89%) | 9 (8%)   | 4 (4%)   | 6           | 53 |
| 17  | Q     | 99/101 (98%)  | 82 (83%)  | 11 (11%) | 6 (6%)   | 2           | 34 |
| 18  | R     | 111/113 (98%) | 99 (89%)  | 8 (7%)   | 4 (4%)   | 5           | 52 |
| 19  | S     | 90/96 (94%)   | 77 (86%)  | 11 (12%) | 2 (2%)   | 10          | 64 |
| 20  | T     | 100/110 (91%) | 71 (71%)  | 13 (13%) | 16 (16%) | 0           | 6  |

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| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|-----------|----------|-------------|-----|
| 21  | U     | 181/206 (88%)   | 126 (70%)  | 34 (19%)  | 21 (12%) | 1           | 13  |
| 22  | V     | 80/85 (94%)     | 65 (81%)   | 14 (18%)  | 1 (1%)   | 18          | 75  |
| 23  | W     | 95/98 (97%)     | 76 (80%)   | 10 (10%)  | 9 (10%)  | 1           | 19  |
| 24  | X     | 67/72 (93%)     | 53 (79%)   | 9 (13%)   | 5 (8%)   | 2           | 27  |
| 25  | Y     | 57/60 (95%)     | 52 (91%)   | 3 (5%)    | 2 (4%)   | 6           | 53  |
| 26  | Z     | 69/71 (97%)     | 35 (51%)   | 18 (26%)  | 16 (23%) | 0           | 2   |
| 27  | a     | 57/60 (95%)     | 47 (82%)   | 7 (12%)   | 3 (5%)   | 3           | 38  |
| 28  | b     | 47/54 (87%)     | 23 (49%)   | 13 (28%)  | 11 (23%) | 0           | 1   |
| 29  | c     | 47/49 (96%)     | 45 (96%)   | 1 (2%)    | 1 (2%)   | 11          | 65  |
| 30  | d     | 62/65 (95%)     | 51 (82%)   | 6 (10%)   | 5 (8%)   | 1           | 24  |
| 31  | e     | 35/37 (95%)     | 35 (100%)  | 0         | 0        | 100         | 100 |
| 32  | f     | 7/12 (58%)      | 5 (71%)    | 2 (29%)   | 0        | 100         | 100 |
| All | All   | 3386/3538 (96%) | 2654 (78%) | 462 (14%) | 270 (8%) | 1           | 25  |

All (270) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C     | 26  | LYS  |
| 3   | C     | 122 | ASP  |
| 3   | C     | 242 | ARG  |
| 4   | D     | 53  | PRO  |
| 4   | D     | 63  | LEU  |
| 4   | D     | 68  | ALA  |
| 4   | D     | 71  | GLY  |
| 4   | D     | 93  | VAL  |
| 7   | G     | 12  | PRO  |
| 7   | G     | 86  | GLU  |
| 7   | G     | 126 | PRO  |
| 7   | G     | 154 | PRO  |
| 7   | G     | 168 | PRO  |
| 7   | G     | 169 | VAL  |
| 8   | H     | 115 | ALA  |
| 8   | H     | 133 | HIS  |
| 9   | I     | 9   | VAL  |
| 9   | I     | 22  | THR  |
| 9   | I     | 96  | GLU  |
| 9   | I     | 131 | GLN  |
| 10  | J     | 5   | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11  | K     | 6   | LEU  |
| 11  | K     | 10  | PRO  |
| 11  | K     | 11  | GLY  |
| 11  | K     | 15  | ARG  |
| 11  | K     | 65  | ARG  |
| 11  | K     | 95  | VAL  |
| 11  | K     | 141 | ALA  |
| 11  | K     | 148 | LEU  |
| 12  | L     | 22  | LYS  |
| 12  | L     | 66  | ILE  |
| 12  | L     | 78  | PRO  |
| 12  | L     | 90  | VAL  |
| 12  | L     | 139 | GLU  |
| 13  | M     | 3   | HIS  |
| 13  | M     | 4   | LEU  |
| 14  | N     | 57  | LYS  |
| 14  | N     | 88  | ASP  |
| 14  | N     | 89  | ARG  |
| 15  | O     | 2   | ASN  |
| 15  | O     | 3   | ARG  |
| 15  | O     | 106 | SER  |
| 15  | O     | 112 | ARG  |
| 15  | O     | 124 | ASP  |
| 16  | P     | 91  | ASP  |
| 17  | Q     | 48  | GLY  |
| 17  | Q     | 50  | PRO  |
| 17  | Q     | 100 | ARG  |
| 18  | R     | 111 | HIS  |
| 20  | T     | 3   | VAL  |
| 20  | T     | 50  | ARG  |
| 20  | T     | 57  | GLN  |
| 20  | T     | 77  | PRO  |
| 20  | T     | 78  | ALA  |
| 21  | U     | 13  | GLU  |
| 21  | U     | 111 | VAL  |
| 24  | X     | 47  | ASN  |
| 24  | X     | 48  | HIS  |
| 24  | X     | 70  | GLN  |
| 24  | X     | 71  | ASN  |
| 26  | Z     | 16  | CYS  |
| 26  | Z     | 18  | CYS  |
| 26  | Z     | 40  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 26  | Z     | 43  | TYR  |
| 26  | Z     | 49  | PHE  |
| 26  | Z     | 50  | VAL  |
| 26  | Z     | 53  | GLU  |
| 27  | a     | 4   | HIS  |
| 27  | a     | 53  | ALA  |
| 28  | b     | 15  | GLU  |
| 30  | d     | 34  | TRP  |
| 30  | d     | 52  | LYS  |
| 30  | d     | 62  | LEU  |
| 3   | C     | 32  | SER  |
| 4   | D     | 50  | GLY  |
| 4   | D     | 60  | ASN  |
| 4   | D     | 66  | HIS  |
| 4   | D     | 72  | VAL  |
| 4   | D     | 90  | THR  |
| 4   | D     | 92  | THR  |
| 4   | D     | 187 | ALA  |
| 5   | E     | 17  | ARG  |
| 5   | E     | 67  | GLN  |
| 5   | E     | 73  | ALA  |
| 5   | E     | 89  | VAL  |
| 5   | E     | 134 | GLY  |
| 5   | E     | 198 | ALA  |
| 6   | F     | 4   | ASP  |
| 6   | F     | 5   | VAL  |
| 6   | F     | 14  | GLU  |
| 6   | F     | 96  | ARG  |
| 6   | F     | 137 | GLU  |
| 6   | F     | 146 | TYR  |
| 7   | G     | 137 | ASP  |
| 7   | G     | 153 | LYS  |
| 7   | G     | 155 | SER  |
| 8   | H     | 10  | GLU  |
| 8   | H     | 11  | ASN  |
| 8   | H     | 102 | SER  |
| 8   | H     | 117 | GLU  |
| 8   | H     | 145 | VAL  |
| 11  | K     | 90  | ARG  |
| 11  | K     | 103 | ALA  |
| 11  | K     | 106 | LEU  |
| 12  | L     | 6   | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12  | L     | 25  | ASP  |
| 12  | L     | 27  | VAL  |
| 12  | L     | 133 | ARG  |
| 13  | M     | 107 | ASP  |
| 14  | N     | 4   | LEU  |
| 14  | N     | 107 | GLU  |
| 15  | O     | 37  | GLY  |
| 16  | P     | 90  | VAL  |
| 17  | Q     | 49  | THR  |
| 17  | Q     | 79  | VAL  |
| 19  | S     | 41  | ASN  |
| 20  | T     | 45  | VAL  |
| 20  | T     | 48  | ALA  |
| 20  | T     | 63  | LYS  |
| 21  | U     | 6   | LYS  |
| 21  | U     | 53  | ILE  |
| 21  | U     | 92  | SER  |
| 21  | U     | 153 | SER  |
| 21  | U     | 177 | PRO  |
| 21  | U     | 179 | ASP  |
| 23  | W     | 30  | VAL  |
| 23  | W     | 80  | LEU  |
| 23  | W     | 84  | GLY  |
| 23  | W     | 91  | LYS  |
| 23  | W     | 95  | LEU  |
| 24  | X     | 43  | GLN  |
| 25  | Y     | 26  | LEU  |
| 26  | Z     | 24  | THR  |
| 26  | Z     | 30  | GLU  |
| 26  | Z     | 51  | ASP  |
| 26  | Z     | 66  | SER  |
| 27  | a     | 59  | GLU  |
| 28  | b     | 7   | ILE  |
| 28  | b     | 45  | LYS  |
| 3   | C     | 46  | GLN  |
| 3   | C     | 239 | ARG  |
| 4   | D     | 79  | ARG  |
| 4   | D     | 204 | ALA  |
| 5   | E     | 133 | ASN  |
| 6   | F     | 32  | PRO  |
| 6   | F     | 116 | ASP  |
| 7   | G     | 5   | GLY  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | G     | 8   | PRO  |
| 7   | G     | 27  | LYS  |
| 7   | G     | 55  | PRO  |
| 7   | G     | 87  | LEU  |
| 7   | G     | 138 | LYS  |
| 8   | H     | 15  | VAL  |
| 8   | H     | 118 | LYS  |
| 9   | I     | 8   | GLN  |
| 9   | I     | 23  | LEU  |
| 9   | I     | 95  | PRO  |
| 9   | I     | 130 | HIS  |
| 10  | J     | 97  | ARG  |
| 11  | K     | 29  | LYS  |
| 11  | K     | 67  | MET  |
| 12  | L     | 11  | LYS  |
| 12  | L     | 19  | GLY  |
| 12  | L     | 137 | TYR  |
| 13  | M     | 74  | LYS  |
| 14  | N     | 12  | PHE  |
| 14  | N     | 61  | ASN  |
| 15  | O     | 12  | SER  |
| 15  | O     | 97  | ALA  |
| 16  | P     | 117 | GLN  |
| 20  | T     | 58  | GLY  |
| 21  | U     | 7   | ALA  |
| 21  | U     | 66  | SER  |
| 21  | U     | 116 | VAL  |
| 21  | U     | 119 | GLU  |
| 21  | U     | 152 | ALA  |
| 23  | W     | 76  | ARG  |
| 25  | Y     | 27  | GLY  |
| 28  | b     | 33  | LYS  |
| 28  | b     | 35  | GLU  |
| 28  | b     | 49  | HIS  |
| 30  | d     | 31  | HIS  |
| 30  | d     | 51  | ALA  |
| 3   | C     | 3   | VAL  |
| 3   | C     | 123 | ALA  |
| 3   | C     | 237 | GLU  |
| 4   | D     | 78  | LEU  |
| 5   | E     | 66  | PRO  |
| 5   | E     | 197 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | F     | 36  | LYS  |
| 6   | F     | 86  | MET  |
| 7   | G     | 92  | ILE  |
| 8   | H     | 122 | GLU  |
| 11  | K     | 21  | ARG  |
| 12  | L     | 21  | THR  |
| 12  | L     | 28  | ALA  |
| 12  | L     | 86  | GLY  |
| 12  | L     | 104 | PHE  |
| 12  | L     | 105 | GLU  |
| 13  | M     | 71  | GLN  |
| 14  | N     | 109 | GLY  |
| 15  | O     | 38  | ASN  |
| 15  | O     | 39  | ARG  |
| 16  | P     | 98  | LEU  |
| 18  | R     | 18  | ARG  |
| 18  | R     | 63  | ASP  |
| 18  | R     | 68  | ARG  |
| 19  | S     | 67  | GLY  |
| 20  | T     | 4   | LYS  |
| 20  | T     | 53  | PRO  |
| 20  | T     | 99  | CYS  |
| 21  | U     | 165 | VAL  |
| 28  | b     | 16  | CYS  |
| 29  | c     | 48  | LYS  |
| 3   | C     | 238 | GLY  |
| 4   | D     | 21  | VAL  |
| 4   | D     | 54  | GLN  |
| 5   | E     | 8   | GLN  |
| 6   | F     | 82  | LEU  |
| 7   | G     | 21  | PRO  |
| 7   | G     | 83  | TYR  |
| 8   | H     | 12  | LEU  |
| 8   | H     | 30  | LEU  |
| 9   | I     | 18  | ALA  |
| 9   | I     | 57  | ALA  |
| 9   | I     | 135 | PRO  |
| 14  | N     | 97  | ARG  |
| 14  | N     | 110 | LEU  |
| 20  | T     | 5   | MET  |
| 20  | T     | 39  | VAL  |
| 20  | T     | 41  | GLY  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 20  | T     | 62  | GLU  |
| 21  | U     | 12  | GLY  |
| 21  | U     | 51  | ALA  |
| 21  | U     | 61  | LEU  |
| 21  | U     | 158 | PRO  |
| 21  | U     | 181 | GLU  |
| 22  | V     | 18  | ALA  |
| 23  | W     | 74  | VAL  |
| 23  | W     | 82  | LEU  |
| 26  | Z     | 5   | ILE  |
| 26  | Z     | 23  | GLU  |
| 26  | Z     | 28  | LYS  |
| 26  | Z     | 68  | ARG  |
| 28  | b     | 9   | LEU  |
| 28  | b     | 19  | ARG  |
| 3   | C     | 125 | ILE  |
| 4   | D     | 82  | ARG  |
| 5   | E     | 130 | ALA  |
| 6   | F     | 52  | ILE  |
| 6   | F     | 88  | ILE  |
| 6   | F     | 117 | PHE  |
| 14  | N     | 82  | ILE  |
| 15  | O     | 40  | THR  |
| 21  | U     | 62  | PRO  |
| 21  | U     | 166 | SER  |
| 23  | W     | 55  | GLY  |
| 26  | Z     | 11  | PRO  |
| 28  | b     | 21  | TYR  |
| 28  | b     | 34  | LEU  |
| 4   | D     | 86  | PRO  |
| 7   | G     | 166 | GLY  |
| 12  | L     | 81  | VAL  |
| 3   | C     | 35  | LYS  |
| 8   | H     | 13  | GLY  |
| 9   | I     | 134 | ARG  |
| 15  | O     | 86  | ILE  |
| 5   | E     | 132 | VAL  |
| 17  | Q     | 54  | GLY  |
| 4   | D     | 22  | PRO  |

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. 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 |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 3   | C     | 214/218 (98%)  | 176 (82%) | 38 (18%) | 2           | 17 |
| 4   | D     | 165/166 (99%)  | 126 (76%) | 39 (24%) | 1           | 8  |
| 5   | E     | 161/166 (97%)  | 132 (82%) | 29 (18%) | 2           | 16 |
| 6   | F     | 155/156 (99%)  | 134 (86%) | 21 (14%) | 6           | 32 |
| 7   | G     | 142/148 (96%)  | 120 (84%) | 22 (16%) | 4           | 25 |
| 8   | H     | 122/124 (98%)  | 98 (80%)  | 24 (20%) | 2           | 12 |
| 9   | I     | 117/119 (98%)  | 97 (83%)  | 20 (17%) | 3           | 20 |
| 10  | J     | 100/100 (100%) | 90 (90%)  | 10 (10%) | 11          | 50 |
| 11  | K     | 116/116 (100%) | 86 (74%)  | 30 (26%) | 1           | 6  |
| 12  | L     | 111/111 (100%) | 94 (85%)  | 17 (15%) | 4           | 26 |
| 13  | M     | 101/101 (100%) | 83 (82%)  | 18 (18%) | 2           | 17 |
| 14  | N     | 87/88 (99%)    | 69 (79%)  | 18 (21%) | 2           | 11 |
| 15  | O     | 120/127 (94%)  | 102 (85%) | 18 (15%) | 4           | 27 |
| 16  | P     | 93/94 (99%)    | 79 (85%)  | 14 (15%) | 4           | 27 |
| 17  | Q     | 82/82 (100%)   | 66 (80%)  | 16 (20%) | 2           | 13 |
| 18  | R     | 92/92 (100%)   | 73 (79%)  | 19 (21%) | 2           | 11 |
| 19  | S     | 74/78 (95%)    | 63 (85%)  | 11 (15%) | 4           | 27 |
| 20  | T     | 85/91 (93%)    | 63 (74%)  | 22 (26%) | 1           | 6  |
| 21  | U     | 162/179 (90%)  | 132 (82%) | 30 (18%) | 2           | 15 |
| 22  | V     | 65/67 (97%)    | 60 (92%)  | 5 (8%)   | 18          | 65 |
| 23  | W     | 82/83 (99%)    | 73 (89%)  | 9 (11%)  | 9           | 44 |
| 24  | X     | 64/67 (96%)    | 57 (89%)  | 7 (11%)  | 9           | 45 |
| 25  | Y     | 51/52 (98%)    | 45 (88%)  | 6 (12%)  | 8           | 39 |
| 26  | Z     | 63/63 (100%)   | 45 (71%)  | 18 (29%) | 0           | 4  |
| 27  | a     | 51/52 (98%)    | 36 (71%)  | 15 (29%) | 0           | 4  |
| 28  | b     | 48/52 (92%)    | 35 (73%)  | 13 (27%) | 1           | 5  |
| 29  | c     | 42/42 (100%)   | 34 (81%)  | 8 (19%)  | 2           | 14 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers  | Percentiles |     |
|-----|-------|-----------------|------------|-----------|-------------|-----|
| 30  | d     | 54/55 (98%)     | 44 (82%)   | 10 (18%)  | 2           | 15  |
| 31  | e     | 34/34 (100%)    | 32 (94%)   | 2 (6%)    | 28          | 76  |
| 32  | f     | 5/7 (71%)       | 5 (100%)   | 0         | 100         | 100 |
| All | All   | 2858/2930 (98%) | 2349 (82%) | 509 (18%) | 2           | 17  |

All (509) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C     | 10  | THR  |
| 3   | C     | 17  | THR  |
| 3   | C     | 25  | THR  |
| 3   | C     | 40  | THR  |
| 3   | C     | 43  | ARG  |
| 3   | C     | 44  | ASN  |
| 3   | C     | 46  | GLN  |
| 3   | C     | 49  | ILE  |
| 3   | C     | 61  | LEU  |
| 3   | C     | 65  | ILE  |
| 3   | C     | 69  | ARG  |
| 3   | C     | 71  | ASP  |
| 3   | C     | 73  | VAL  |
| 3   | C     | 83  | GLU  |
| 3   | C     | 87  | ASN  |
| 3   | C     | 88  | ARG  |
| 3   | C     | 95  | LEU  |
| 3   | C     | 103 | ARG  |
| 3   | C     | 105 | ILE  |
| 3   | C     | 106 | ILE  |
| 3   | C     | 111 | LEU  |
| 3   | C     | 150 | LYS  |
| 3   | C     | 155 | LEU  |
| 3   | C     | 157 | ARG  |
| 3   | C     | 173 | VAL  |
| 3   | C     | 192 | THR  |
| 3   | C     | 211 | ARG  |
| 3   | C     | 212 | SER  |
| 3   | C     | 221 | VAL  |
| 3   | C     | 229 | VAL  |
| 3   | C     | 237 | GLU  |
| 3   | C     | 242 | ARG  |
| 3   | C     | 257 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C     | 259 | THR  |
| 3   | C     | 261 | LYS  |
| 3   | C     | 268 | ARG  |
| 3   | C     | 271 | ILE  |
| 3   | C     | 273 | ARG  |
| 4   | D     | 2   | LYS  |
| 4   | D     | 4   | ILE  |
| 4   | D     | 7   | VAL  |
| 4   | D     | 12  | THR  |
| 4   | D     | 13  | ARG  |
| 4   | D     | 16  | ARG  |
| 4   | D     | 26  | ILE  |
| 4   | D     | 27  | LEU  |
| 4   | D     | 33  | VAL  |
| 4   | D     | 34  | VAL  |
| 4   | D     | 38  | THR  |
| 4   | D     | 41  | LYS  |
| 4   | D     | 42  | ASP  |
| 4   | D     | 47  | VAL  |
| 4   | D     | 49  | LEU  |
| 4   | D     | 52  | LEU  |
| 4   | D     | 54  | GLN  |
| 4   | D     | 63  | LEU  |
| 4   | D     | 77  | ILE  |
| 4   | D     | 79  | ARG  |
| 4   | D     | 80  | GLU  |
| 4   | D     | 82  | ARG  |
| 4   | D     | 92  | THR  |
| 4   | D     | 101 | ARG  |
| 4   | D     | 113 | PHE  |
| 4   | D     | 116 | VAL  |
| 4   | D     | 119 | ARG  |
| 4   | D     | 127 | ASP  |
| 4   | D     | 144 | ARG  |
| 4   | D     | 146 | THR  |
| 4   | D     | 167 | VAL  |
| 4   | D     | 175 | VAL  |
| 4   | D     | 179 | GLU  |
| 4   | D     | 181 | LEU  |
| 4   | D     | 184 | VAL  |
| 4   | D     | 197 | ILE  |
| 4   | D     | 200 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | D     | 202 | LYS  |
| 4   | D     | 203 | LYS  |
| 5   | E     | 9   | ILE  |
| 5   | E     | 13  | SER  |
| 5   | E     | 24  | LEU  |
| 5   | E     | 28  | ILE  |
| 5   | E     | 32  | LEU  |
| 5   | E     | 33  | LEU  |
| 5   | E     | 45  | ARG  |
| 5   | E     | 57  | VAL  |
| 5   | E     | 65  | TRP  |
| 5   | E     | 68  | LYS  |
| 5   | E     | 70  | THR  |
| 5   | E     | 74  | ARG  |
| 5   | E     | 77  | ASP  |
| 5   | E     | 78  | ILE  |
| 5   | E     | 84  | VAL  |
| 5   | E     | 104 | LYS  |
| 5   | E     | 107 | LYS  |
| 5   | E     | 117 | ARG  |
| 5   | E     | 127 | GLU  |
| 5   | E     | 149 | ASP  |
| 5   | E     | 158 | THR  |
| 5   | E     | 161 | GLU  |
| 5   | E     | 165 | ARG  |
| 5   | E     | 174 | VAL  |
| 5   | E     | 176 | LEU  |
| 5   | E     | 181 | LEU  |
| 5   | E     | 192 | LEU  |
| 5   | E     | 194 | MET  |
| 5   | E     | 197 | ASP  |
| 6   | F     | 7   | LEU  |
| 6   | F     | 10  | LYS  |
| 6   | F     | 20  | ILE  |
| 6   | F     | 26  | GLN  |
| 6   | F     | 33  | ARG  |
| 6   | F     | 34  | LEU  |
| 6   | F     | 43  | LEU  |
| 6   | F     | 53  | LEU  |
| 6   | F     | 54  | GLU  |
| 6   | F     | 67  | LYS  |
| 6   | F     | 71  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | F     | 88  | ILE  |
| 6   | F     | 94  | LEU  |
| 6   | F     | 98  | ARG  |
| 6   | F     | 116 | ASP  |
| 6   | F     | 118 | ARG  |
| 6   | F     | 133 | LEU  |
| 6   | F     | 147 | ASP  |
| 6   | F     | 159 | VAL  |
| 6   | F     | 167 | GLU  |
| 6   | F     | 174 | GLU  |
| 7   | G     | 3   | ARG  |
| 7   | G     | 4   | ILE  |
| 7   | G     | 7   | LEU  |
| 7   | G     | 9   | ILE  |
| 7   | G     | 27  | LYS  |
| 7   | G     | 42  | ARG  |
| 7   | G     | 43  | VAL  |
| 7   | G     | 51  | ARG  |
| 7   | G     | 59  | ARG  |
| 7   | G     | 64  | LEU  |
| 7   | G     | 77  | LYS  |
| 7   | G     | 81  | GLU  |
| 7   | G     | 88  | LEU  |
| 7   | G     | 89  | ILE  |
| 7   | G     | 105 | LEU  |
| 7   | G     | 107 | VAL  |
| 7   | G     | 127 | GLU  |
| 7   | G     | 132 | ARG  |
| 7   | G     | 152 | ARG  |
| 7   | G     | 153 | LYS  |
| 7   | G     | 158 | HIS  |
| 7   | G     | 169 | VAL  |
| 8   | H     | 1   | MET  |
| 8   | H     | 2   | LYS  |
| 8   | H     | 9   | LEU  |
| 8   | H     | 10  | GLU  |
| 8   | H     | 27  | ARG  |
| 8   | H     | 31  | LEU  |
| 8   | H     | 33  | ARG  |
| 8   | H     | 38  | LEU  |
| 8   | H     | 44  | LEU  |
| 8   | H     | 56  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8   | H     | 57  | ARG  |
| 8   | H     | 70  | GLU  |
| 8   | H     | 72  | LEU  |
| 8   | H     | 81  | VAL  |
| 8   | H     | 92  | VAL  |
| 8   | H     | 101 | LEU  |
| 8   | H     | 113 | ARG  |
| 8   | H     | 128 | LEU  |
| 8   | H     | 129 | THR  |
| 8   | H     | 130 | TYR  |
| 8   | H     | 131 | LYS  |
| 8   | H     | 135 | GLU  |
| 8   | H     | 142 | VAL  |
| 8   | H     | 145 | VAL  |
| 9   | I     | 1   | MET  |
| 9   | I     | 2   | LYS  |
| 9   | I     | 5   | VAL  |
| 9   | I     | 7   | LYS  |
| 9   | I     | 12  | ARG  |
| 9   | I     | 32  | THR  |
| 9   | I     | 34  | LEU  |
| 9   | I     | 43  | THR  |
| 9   | I     | 48  | MET  |
| 9   | I     | 60  | ILE  |
| 9   | I     | 61  | ARG  |
| 9   | I     | 62  | VAL  |
| 9   | I     | 87  | LEU  |
| 9   | I     | 90  | MET  |
| 9   | I     | 96  | GLU  |
| 9   | I     | 98  | VAL  |
| 9   | I     | 109 | LYS  |
| 9   | I     | 120 | LEU  |
| 9   | I     | 127 | ASP  |
| 9   | I     | 136 | GLU  |
| 10  | J     | 3   | GLN  |
| 10  | J     | 9   | GLU  |
| 10  | J     | 19  | ILE  |
| 10  | J     | 24  | VAL  |
| 10  | J     | 31  | LYS  |
| 10  | J     | 49  | ARG  |
| 10  | J     | 53  | LYS  |
| 10  | J     | 69  | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10  | J     | 91  | LEU  |
| 10  | J     | 102 | VAL  |
| 11  | K     | 5   | ASP  |
| 11  | K     | 6   | LEU  |
| 11  | K     | 14  | LYS  |
| 11  | K     | 15  | ARG  |
| 11  | K     | 16  | ARG  |
| 11  | K     | 19  | VAL  |
| 11  | K     | 21  | ARG  |
| 11  | K     | 30  | THR  |
| 11  | K     | 36  | LYS  |
| 11  | K     | 41  | ARG  |
| 11  | K     | 45  | LEU  |
| 11  | K     | 50  | ARG  |
| 11  | K     | 56  | SER  |
| 11  | K     | 61  | ARG  |
| 11  | K     | 62  | LEU  |
| 11  | K     | 64  | LYS  |
| 11  | K     | 70  | GLN  |
| 11  | K     | 71  | VAL  |
| 11  | K     | 75  | ILE  |
| 11  | K     | 81  | GLN  |
| 11  | K     | 88  | LEU  |
| 11  | K     | 91  | PHE  |
| 11  | K     | 100 | LEU  |
| 11  | K     | 105 | LEU  |
| 11  | K     | 107 | LYS  |
| 11  | K     | 112 | LEU  |
| 11  | K     | 133 | SER  |
| 11  | K     | 138 | LEU  |
| 11  | K     | 144 | GLU  |
| 11  | K     | 146 | VAL  |
| 12  | L     | 17  | LEU  |
| 12  | L     | 26  | TYR  |
| 12  | L     | 27  | VAL  |
| 12  | L     | 35  | VAL  |
| 12  | L     | 45  | GLN  |
| 12  | L     | 54  | MET  |
| 12  | L     | 60  | ARG  |
| 12  | L     | 79  | LEU  |
| 12  | L     | 80  | GLU  |
| 12  | L     | 81  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12  | L     | 82  | ARG  |
| 12  | L     | 83  | MET  |
| 12  | L     | 85  | LYS  |
| 12  | L     | 96  | VAL  |
| 12  | L     | 112 | GLU  |
| 12  | L     | 135 | ASP  |
| 12  | L     | 139 | GLU  |
| 13  | M     | 1   | MET  |
| 13  | M     | 6   | SER  |
| 13  | M     | 9   | LYS  |
| 13  | M     | 18  | LEU  |
| 13  | M     | 29  | LEU  |
| 13  | M     | 35  | THR  |
| 13  | M     | 44  | LEU  |
| 13  | M     | 63  | ARG  |
| 13  | M     | 71  | GLN  |
| 13  | M     | 75  | LEU  |
| 13  | M     | 79  | LEU  |
| 13  | M     | 91  | GLN  |
| 13  | M     | 95  | THR  |
| 13  | M     | 100 | LEU  |
| 13  | M     | 104 | ARG  |
| 13  | M     | 105 | ARG  |
| 13  | M     | 117 | VAL  |
| 13  | M     | 118 | GLU  |
| 14  | N     | 3   | ARG  |
| 14  | N     | 4   | LEU  |
| 14  | N     | 12  | PHE  |
| 14  | N     | 17  | ARG  |
| 14  | N     | 20  | ARG  |
| 14  | N     | 27  | SER  |
| 14  | N     | 39  | ILE  |
| 14  | N     | 44  | LYS  |
| 14  | N     | 50  | SER  |
| 14  | N     | 54  | LEU  |
| 14  | N     | 56  | LEU  |
| 14  | N     | 57  | LYS  |
| 14  | N     | 58  | LEU  |
| 14  | N     | 59  | LYS  |
| 14  | N     | 98  | VAL  |
| 14  | N     | 101 | LEU  |
| 14  | N     | 103 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 14  | N     | 106 | ARG  |
| 15  | O     | 18  | ASP  |
| 15  | O     | 27  | THR  |
| 15  | O     | 30  | VAL  |
| 15  | O     | 41  | ARG  |
| 15  | O     | 42  | ILE  |
| 15  | O     | 50  | ILE  |
| 15  | O     | 51  | ARG  |
| 15  | O     | 62  | THR  |
| 15  | O     | 65  | LYS  |
| 15  | O     | 74  | ARG  |
| 15  | O     | 88  | ILE  |
| 15  | O     | 89  | VAL  |
| 15  | O     | 99  | LEU  |
| 15  | O     | 105 | LEU  |
| 15  | O     | 107 | ASP  |
| 15  | O     | 112 | ARG  |
| 15  | O     | 125 | ARG  |
| 15  | O     | 128 | GLU  |
| 16  | P     | 52  | ARG  |
| 16  | P     | 55  | ARG  |
| 16  | P     | 59  | ARG  |
| 16  | P     | 60  | LEU  |
| 16  | P     | 64  | ARG  |
| 16  | P     | 69  | CYS  |
| 16  | P     | 74  | LEU  |
| 16  | P     | 90  | VAL  |
| 16  | P     | 92  | ARG  |
| 16  | P     | 98  | LEU  |
| 16  | P     | 108 | GLU  |
| 16  | P     | 111 | GLU  |
| 16  | P     | 114 | LYS  |
| 16  | P     | 117 | GLN  |
| 17  | Q     | 13  | ARG  |
| 17  | Q     | 19  | LYS  |
| 17  | Q     | 21  | ARG  |
| 17  | Q     | 22  | VAL  |
| 17  | Q     | 24  | LYS  |
| 17  | Q     | 35  | LEU  |
| 17  | Q     | 37  | VAL  |
| 17  | Q     | 45  | THR  |
| 17  | Q     | 47  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 17  | Q     | 57  | VAL  |
| 17  | Q     | 61  | VAL  |
| 17  | Q     | 62  | LEU  |
| 17  | Q     | 64  | HIS  |
| 17  | Q     | 78  | LYS  |
| 17  | Q     | 79  | VAL  |
| 17  | Q     | 99  | ILE  |
| 18  | R     | 11  | ARG  |
| 18  | R     | 16  | LYS  |
| 18  | R     | 18  | ARG  |
| 18  | R     | 19  | LEU  |
| 18  | R     | 20  | VAL  |
| 18  | R     | 23  | LEU  |
| 18  | R     | 27  | LYS  |
| 18  | R     | 30  | GLU  |
| 18  | R     | 40  | ASN  |
| 18  | R     | 51  | LEU  |
| 18  | R     | 60  | ASN  |
| 18  | R     | 63  | ASP  |
| 18  | R     | 67  | ASP  |
| 18  | R     | 76  | VAL  |
| 18  | R     | 82  | LEU  |
| 18  | R     | 92  | ARG  |
| 18  | R     | 100 | THR  |
| 18  | R     | 106 | ILE  |
| 18  | R     | 107 | LEU  |
| 19  | S     | 12  | VAL  |
| 19  | S     | 23  | GLU  |
| 19  | S     | 27  | THR  |
| 19  | S     | 30  | VAL  |
| 19  | S     | 35  | THR  |
| 19  | S     | 49  | VAL  |
| 19  | S     | 55  | ASN  |
| 19  | S     | 65  | ARG  |
| 19  | S     | 70  | LEU  |
| 19  | S     | 80  | ILE  |
| 19  | S     | 81  | VAL  |
| 20  | T     | 2   | ARG  |
| 20  | T     | 13  | VAL  |
| 20  | T     | 14  | LEU  |
| 20  | T     | 27  | VAL  |
| 20  | T     | 34  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 20  | T     | 37  | VAL  |
| 20  | T     | 38  | ILE  |
| 20  | T     | 43  | ASN  |
| 20  | T     | 45  | VAL  |
| 20  | T     | 55  | TYR  |
| 20  | T     | 57  | GLN  |
| 20  | T     | 61  | ILE  |
| 20  | T     | 67  | LEU  |
| 20  | T     | 70  | SER  |
| 20  | T     | 75  | ILE  |
| 20  | T     | 76  | CYS  |
| 20  | T     | 87  | LYS  |
| 20  | T     | 90  | LEU  |
| 20  | T     | 95  | LYS  |
| 20  | T     | 96  | ILE  |
| 20  | T     | 97  | ARG  |
| 20  | T     | 102 | CYS  |
| 21  | U     | 2   | GLU  |
| 21  | U     | 5   | LEU  |
| 21  | U     | 19  | ARG  |
| 21  | U     | 20  | ARG  |
| 21  | U     | 52  | SER  |
| 21  | U     | 53  | ILE  |
| 21  | U     | 60  | GLU  |
| 21  | U     | 70  | LEU  |
| 21  | U     | 71  | VAL  |
| 21  | U     | 81  | ARG  |
| 21  | U     | 87  | ASP  |
| 21  | U     | 91  | LEU  |
| 21  | U     | 92  | SER  |
| 21  | U     | 93  | ASP  |
| 21  | U     | 94  | GLU  |
| 21  | U     | 107 | THR  |
| 21  | U     | 112 | ARG  |
| 21  | U     | 117 | LEU  |
| 21  | U     | 121 | HIS  |
| 21  | U     | 128 | VAL  |
| 21  | U     | 131 | ARG  |
| 21  | U     | 142 | SER  |
| 21  | U     | 145 | GLU  |
| 21  | U     | 150 | LEU  |
| 21  | U     | 151 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 21  | U     | 163 | LEU  |
| 21  | U     | 168 | GLU  |
| 21  | U     | 174 | VAL  |
| 21  | U     | 182 | LYS  |
| 21  | U     | 183 | LEU  |
| 22  | V     | 7   | LEU  |
| 22  | V     | 10  | THR  |
| 22  | V     | 36  | ILE  |
| 22  | V     | 53  | MET  |
| 22  | V     | 74  | ARG  |
| 23  | W     | 21  | ARG  |
| 23  | W     | 41  | ARG  |
| 23  | W     | 51  | VAL  |
| 23  | W     | 62  | VAL  |
| 23  | W     | 78  | LYS  |
| 23  | W     | 80  | LEU  |
| 23  | W     | 90  | ILE  |
| 23  | W     | 91  | LYS  |
| 23  | W     | 92  | LYS  |
| 24  | X     | 17  | SER  |
| 24  | X     | 24  | LEU  |
| 24  | X     | 27  | GLU  |
| 24  | X     | 32  | LEU  |
| 24  | X     | 50  | ILE  |
| 24  | X     | 53  | LEU  |
| 24  | X     | 62  | THR  |
| 25  | Y     | 6   | VAL  |
| 25  | Y     | 8   | LEU  |
| 25  | Y     | 18  | ASP  |
| 25  | Y     | 32  | GLN  |
| 25  | Y     | 40  | THR  |
| 25  | Y     | 56  | VAL  |
| 26  | Z     | 13  | ARG  |
| 26  | Z     | 15  | ILE  |
| 26  | Z     | 23  | GLU  |
| 26  | Z     | 33  | VAL  |
| 26  | Z     | 34  | GLU  |
| 26  | Z     | 37  | SER  |
| 26  | Z     | 42  | PHE  |
| 26  | Z     | 48  | ARG  |
| 26  | Z     | 49  | PHE  |
| 26  | Z     | 50  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 26  | Z     | 52  | THR  |
| 26  | Z     | 57  | GLU  |
| 26  | Z     | 61  | ARG  |
| 26  | Z     | 62  | ARG  |
| 26  | Z     | 63  | TYR  |
| 26  | Z     | 66  | SER  |
| 26  | Z     | 67  | TYR  |
| 26  | Z     | 68  | ARG  |
| 27  | a     | 4   | HIS  |
| 27  | a     | 6   | VAL  |
| 27  | a     | 11  | THR  |
| 27  | a     | 21  | SER  |
| 27  | a     | 23  | HIS  |
| 27  | a     | 25  | LEU  |
| 27  | a     | 29  | THR  |
| 27  | a     | 36  | CYS  |
| 27  | a     | 40  | LYS  |
| 27  | a     | 46  | CYS  |
| 27  | a     | 51  | TYR  |
| 27  | a     | 55  | ARG  |
| 27  | a     | 56  | LYS  |
| 27  | a     | 58  | LEU  |
| 27  | a     | 60  | VAL  |
| 28  | b     | 6   | ARG  |
| 28  | b     | 8   | LYS  |
| 28  | b     | 9   | LEU  |
| 28  | b     | 10  | LEU  |
| 28  | b     | 11  | LEU  |
| 28  | b     | 17  | LYS  |
| 28  | b     | 19  | ARG  |
| 28  | b     | 23  | THR  |
| 28  | b     | 27  | LYS  |
| 28  | b     | 30  | THR  |
| 28  | b     | 34  | LEU  |
| 28  | b     | 37  | ARG  |
| 28  | b     | 44  | ARG  |
| 29  | c     | 1   | MET  |
| 29  | c     | 2   | LYS  |
| 29  | c     | 4   | THR  |
| 29  | c     | 9   | ARG  |
| 29  | c     | 10  | ARG  |
| 29  | c     | 14  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 29  | c     | 43  | THR  |
| 29  | c     | 46  | VAL  |
| 30  | d     | 14  | VAL  |
| 30  | d     | 15  | LYS  |
| 30  | d     | 34  | TRP  |
| 30  | d     | 35  | GLN  |
| 30  | d     | 44  | LYS  |
| 30  | d     | 47  | LYS  |
| 30  | d     | 49  | VAL  |
| 30  | d     | 52  | LYS  |
| 30  | d     | 64  | TYR  |
| 30  | d     | 65  | GLU  |
| 31  | e     | 1   | MET  |
| 31  | e     | 29  | ASN  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 14  | N     | 34  | HIS  |
| 19  | S     | 55  | ASN  |
| 27  | a     | 22  | HIS  |
| 31  | e     | 29  | ASN  |
| 31  | e     | 32  | HIS  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | A     | 2879/2915 (98%) | 567 (19%)         | 57 (1%)         |
| 2   | B     | 119/122 (97%)   | 21 (17%)          | 1 (0%)          |
| All | All   | 2998/3037 (98%) | 588 (19%)         | 58 (1%)         |

All (588) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 9   | U    |
| 1   | A     | 15  | G    |
| 1   | A     | 28  | A    |
| 1   | A     | 34  | C    |
| 1   | A     | 35  | G    |
| 1   | A     | 46  | C    |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | A     | 51     | G    |
| 1   | A     | 55     | G    |
| 1   | A     | 72     | U    |
| 1   | A     | 74     | A    |
| 1   | A     | 75     | G    |
| 1   | A     | 96     | G    |
| 1   | A     | 101    | G    |
| 1   | A     | 102    | G    |
| 1   | A     | 103    | A    |
| 1   | A     | 118    | A    |
| 1   | A     | 120    | U    |
| 1   | A     | 131    | G    |
| 1   | A     | 138    | G    |
| 1   | A     | 161    | U    |
| 1   | A     | 177    | G    |
| 1   | A     | 181    | A    |
| 1   | A     | 196    | A    |
| 1   | A     | 199    | A    |
| 1   | A     | 206    | U    |
| 1   | A     | 214    | G    |
| 1   | A     | 215    | G    |
| 1   | A     | 216    | A    |
| 1   | A     | 221    | A    |
| 1   | A     | 222    | A    |
| 1   | A     | 223    | A    |
| 1   | A     | 224    | G    |
| 1   | A     | 226    | G    |
| 1   | A     | 228    | A    |
| 1   | A     | 229    | A    |
| 1   | A     | 230    | U    |
| 1   | A     | 232    | G    |
| 1   | A     | 233    | A    |
| 1   | A     | 242    | G    |
| 1   | A     | 243    | U    |
| 1   | A     | 248    | G    |
| 1   | A     | 249    | C    |
| 1   | A     | 250    | G    |
| 1   | A     | 252    | G    |
| 1   | A     | 265    | A    |
| 1   | A     | 266    | G    |
| 1   | A     | 269    | U    |
| 1   | A     | 270(L) | U    |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | A     | 270(M) | U    |
| 1   | A     | 270(N) | G    |
| 1   | A     | 270(P) | C    |
| 1   | A     | 271(A) | C    |
| 1   | A     | 271(B) | G    |
| 1   | A     | 271(C) | U    |
| 1   | A     | 271    | G    |
| 1   | A     | 275    | G    |
| 1   | A     | 276    | A    |
| 1   | A     | 277    | C    |
| 1   | A     | 278    | A    |
| 1   | A     | 279    | C    |
| 1   | A     | 299    | A    |
| 1   | A     | 300    | A    |
| 1   | A     | 311    | A    |
| 1   | A     | 317    | G    |
| 1   | A     | 323    | G    |
| 1   | A     | 324    | A    |
| 1   | A     | 329    | G    |
| 1   | A     | 330    | A    |
| 1   | A     | 342    | G    |
| 1   | A     | 346    | A    |
| 1   | A     | 352    | G    |
| 1   | A     | 364    | C    |
| 1   | A     | 371    | A    |
| 1   | A     | 372    | G    |
| 1   | A     | 373    | U    |
| 1   | A     | 386    | G    |
| 1   | A     | 404    | C    |
| 1   | A     | 405    | U    |
| 1   | A     | 411    | G    |
| 1   | A     | 412    | A    |
| 1   | A     | 428    | A    |
| 1   | A     | 444    | C    |
| 1   | A     | 448    | U    |
| 1   | A     | 454    | A    |
| 1   | A     | 457    | A    |
| 1   | A     | 470    | A    |
| 1   | A     | 481    | G    |
| 1   | A     | 504    | U    |
| 1   | A     | 505    | A    |
| 1   | A     | 509    | C    |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | A     | 513    | A    |
| 1   | A     | 527    | C    |
| 1   | A     | 529    | A    |
| 1   | A     | 531    | C    |
| 1   | A     | 532    | A    |
| 1   | A     | 533    | G    |
| 1   | A     | 537    | C    |
| 1   | A     | 539    | G    |
| 1   | A     | 540    | G    |
| 1   | A     | 546    | C    |
| 1   | A     | 547    | A    |
| 1   | A     | 556    | G    |
| 1   | A     | 563    | G    |
| 1   | A     | 568    | U    |
| 1   | A     | 573    | G    |
| 1   | A     | 574    | C    |
| 1   | A     | 575    | A    |
| 1   | A     | 588    | U    |
| 1   | A     | 603    | A    |
| 1   | A     | 607    | U    |
| 1   | A     | 614    | U    |
| 1   | A     | 615    | G    |
| 1   | A     | 617    | G    |
| 1   | A     | 621    | A    |
| 1   | A     | 626    | U    |
| 1   | A     | 627    | A    |
| 1   | A     | 637    | A    |
| 1   | A     | 638    | G    |
| 1   | A     | 645    | C    |
| 1   | A     | 646    | A    |
| 1   | A     | 651    | G    |
| 1   | A     | 652    | C    |
| 1   | A     | 654    | A    |
| 1   | A     | 654(A) | G    |
| 1   | A     | 668    | G    |
| 1   | A     | 669    | G    |
| 1   | A     | 670    | A    |
| 1   | A     | 686    | G    |
| 1   | A     | 702    | G    |
| 1   | A     | 717    | G    |
| 1   | A     | 721    | C    |
| 1   | A     | 722    | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 730 | C    |
| 1   | A     | 776 | G    |
| 1   | A     | 782 | A    |
| 1   | A     | 784 | A    |
| 1   | A     | 785 | G    |
| 1   | A     | 789 | A    |
| 1   | A     | 790 | C    |
| 1   | A     | 805 | G    |
| 1   | A     | 812 | C    |
| 1   | A     | 819 | A    |
| 1   | A     | 827 | U    |
| 1   | A     | 828 | U    |
| 1   | A     | 846 | C    |
| 1   | A     | 847 | U    |
| 1   | A     | 856 | C    |
| 1   | A     | 857 | C    |
| 1   | A     | 859 | G    |
| 1   | A     | 860 | U    |
| 1   | A     | 869 | G    |
| 1   | A     | 872 | A    |
| 1   | A     | 881 | G    |
| 1   | A     | 884 | C    |
| 1   | A     | 885 | C    |
| 1   | A     | 886 | C    |
| 1   | A     | 888 | C    |
| 1   | A     | 889 | C    |
| 1   | A     | 893 | C    |
| 1   | A     | 896 | A    |
| 1   | A     | 897 | C    |
| 1   | A     | 899 | A    |
| 1   | A     | 900 | A    |
| 1   | A     | 901 | A    |
| 1   | A     | 904 | C    |
| 1   | A     | 907 | U    |
| 1   | A     | 910 | A    |
| 1   | A     | 917 | A    |
| 1   | A     | 932 | G    |
| 1   | A     | 941 | A    |
| 1   | A     | 945 | A    |
| 1   | A     | 946 | G    |
| 1   | A     | 961 | C    |
| 1   | A     | 974 | G    |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | A     | 974(A) | C    |
| 1   | A     | 975    | G    |
| 1   | A     | 980    | A    |
| 1   | A     | 983    | A    |
| 1   | A     | 996    | A    |
| 1   | A     | 1003   | G    |
| 1   | A     | 1011   | G    |
| 1   | A     | 1012   | U    |
| 1   | A     | 1013   | C    |
| 1   | A     | 1015   | G    |
| 1   | A     | 1017   | G    |
| 1   | A     | 1020   | A    |
| 1   | A     | 1023   | U    |
| 1   | A     | 1025   | G    |
| 1   | A     | 1026   | U    |
| 1   | A     | 1027   | A    |
| 1   | A     | 1033   | U    |
| 1   | A     | 1044   | G    |
| 1   | A     | 1045   | A    |
| 1   | A     | 1046   | A    |
| 1   | A     | 1050   | A    |
| 1   | A     | 1054   | A    |
| 1   | A     | 1055   | G    |
| 1   | A     | 1057   | A    |
| 1   | A     | 1059   | G    |
| 1   | A     | 1060   | U    |
| 1   | A     | 1061   | U    |
| 1   | A     | 1065   | U    |
| 1   | A     | 1066   | U    |
| 1   | A     | 1067   | A    |
| 1   | A     | 1068   | G    |
| 1   | A     | 1069   | A    |
| 1   | A     | 1070   | A    |
| 1   | A     | 1071   | G    |
| 1   | A     | 1076   | C    |
| 1   | A     | 1077   | A    |
| 1   | A     | 1078   | U    |
| 1   | A     | 1079   | C    |
| 1   | A     | 1080   | C    |
| 1   | A     | 1082   | U    |
| 1   | A     | 1083   | U    |
| 1   | A     | 1084   | A    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 1   | A     | 1085    | A    |
| 1   | A     | 1086    | A    |
| 1   | A     | 1087    | G    |
| 1   | A     | 1088    | A    |
| 1   | A     | 1091    | G    |
| 1   | A     | 1093    | G    |
| 1   | A     | 1095    | A    |
| 1   | A     | 1096    | A    |
| 1   | A     | 1104    | C    |
| 1   | A     | 1110    | G    |
| 1   | A     | 1111    | A    |
| 1   | A     | 1112    | G    |
| 1   | A     | 1122    | G    |
| 1   | A     | 1130    | U    |
| 1   | A     | 1131    | G    |
| 1   | A     | 1135    | C    |
| 1   | A     | 1136    | G    |
| 1   | A     | 1142    | U    |
| 1   | A     | 1142(A) | A    |
| 1   | A     | 1151    | G    |
| 1   | A     | 1155    | A    |
| 1   | A     | 1170    | G    |
| 1   | A     | 1173    | G    |
| 1   | A     | 1174    | A    |
| 1   | A     | 1175    | U    |
| 1   | A     | 1176    | G    |
| 1   | A     | 1178    | C    |
| 1   | A     | 1179    | C    |
| 1   | A     | 1180    | C    |
| 1   | A     | 1183    | G    |
| 1   | A     | 1195    | G    |
| 1   | A     | 1204    | A    |
| 1   | A     | 1205    | U    |
| 1   | A     | 1206    | G    |
| 1   | A     | 1210    | A    |
| 1   | A     | 1211    | U    |
| 1   | A     | 1220    | A    |
| 1   | A     | 1221    | C    |
| 1   | A     | 1236    | G    |
| 1   | A     | 1238    | G    |
| 1   | A     | 1252    | G    |
| 1   | A     | 1253    | A    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 1   | A     | 1256    | G    |
| 1   | A     | 1265    | A    |
| 1   | A     | 1271    | G    |
| 1   | A     | 1272    | A    |
| 1   | A     | 1273    | U    |
| 1   | A     | 1288    | U    |
| 1   | A     | 1300    | U    |
| 1   | A     | 1301    | A    |
| 1   | A     | 1312    | U    |
| 1   | A     | 1313    | U    |
| 1   | A     | 1314    | C    |
| 1   | A     | 1321    | A    |
| 1   | A     | 1329    | U    |
| 1   | A     | 1332    | G    |
| 1   | A     | 1349    | A    |
| 1   | A     | 1365    | A    |
| 1   | A     | 1368    | G    |
| 1   | A     | 1370    | C    |
| 1   | A     | 1379    | A    |
| 1   | A     | 1380    | G    |
| 1   | A     | 1384    | A    |
| 1   | A     | 1385    | G    |
| 1   | A     | 1386    | C    |
| 1   | A     | 1407    | C    |
| 1   | A     | 1408    | C    |
| 1   | A     | 1411    | C    |
| 1   | A     | 1412    | A    |
| 1   | A     | 1416    | G    |
| 1   | A     | 1419    | A    |
| 1   | A     | 1420    | U    |
| 1   | A     | 1421    | G    |
| 1   | A     | 1428    | C    |
| 1   | A     | 1444(A) | A    |
| 1   | A     | 1445    | C    |
| 1   | A     | 1449    | A    |
| 1   | A     | 1449(A) | G    |
| 1   | A     | 1455    | G    |
| 1   | A     | 1458    | C    |
| 1   | A     | 1460    | A    |
| 1   | A     | 1461    | G    |
| 1   | A     | 1467    | C    |
| 1   | A     | 1471    | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1482 | U    |
| 1   | A     | 1483 | G    |
| 1   | A     | 1485 | G    |
| 1   | A     | 1493 | C    |
| 1   | A     | 1497 | U    |
| 1   | A     | 1505 | C    |
| 1   | A     | 1506 | C    |
| 1   | A     | 1507 | A    |
| 1   | A     | 1508 | A    |
| 1   | A     | 1510 | A    |
| 1   | A     | 1514 | U    |
| 1   | A     | 1519 | G    |
| 1   | A     | 1522 | G    |
| 1   | A     | 1534 | G    |
| 1   | A     | 1535 | U    |
| 1   | A     | 1536 | A    |
| 1   | A     | 1537 | C    |
| 1   | A     | 1538 | G    |
| 1   | A     | 1543 | A    |
| 1   | A     | 1544 | C    |
| 1   | A     | 1545 | A    |
| 1   | A     | 1547 | C    |
| 1   | A     | 1558 | A    |
| 1   | A     | 1559 | G    |
| 1   | A     | 1569 | A    |
| 1   | A     | 1578 | U    |
| 1   | A     | 1579 | A    |
| 1   | A     | 1580 | A    |
| 1   | A     | 1581 | G    |
| 1   | A     | 1585 | C    |
| 1   | A     | 1586 | A    |
| 1   | A     | 1598 | C    |
| 1   | A     | 1608 | A    |
| 1   | A     | 1609 | A    |
| 1   | A     | 1610 | A    |
| 1   | A     | 1616 | A    |
| 1   | A     | 1617 | C    |
| 1   | A     | 1618 | A    |
| 1   | A     | 1640 | C    |
| 1   | A     | 1646 | C    |
| 1   | A     | 1648 | C    |
| 1   | A     | 1654 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1667 | G    |
| 1   | A     | 1674 | G    |
| 1   | A     | 1675 | C    |
| 1   | A     | 1688 | U    |
| 1   | A     | 1695 | G    |
| 1   | A     | 1725 | G    |
| 1   | A     | 1729 | A    |
| 1   | A     | 1730 | U    |
| 1   | A     | 1731 | G    |
| 1   | A     | 1732 | A    |
| 1   | A     | 1733 | G    |
| 1   | A     | 1742 | C    |
| 1   | A     | 1743 | G    |
| 1   | A     | 1756 | G    |
| 1   | A     | 1763 | G    |
| 1   | A     | 1764 | G    |
| 1   | A     | 1773 | A    |
| 1   | A     | 1780 | A    |
| 1   | A     | 1782 | C    |
| 1   | A     | 1791 | A    |
| 1   | A     | 1799 | G    |
| 1   | A     | 1800 | C    |
| 1   | A     | 1801 | G    |
| 1   | A     | 1816 | G    |
| 1   | A     | 1820 | U    |
| 1   | A     | 1829 | A    |
| 1   | A     | 1835 | G    |
| 1   | A     | 1847 | A    |
| 1   | A     | 1848 | A    |
| 1   | A     | 1858 | G    |
| 1   | A     | 1869 | G    |
| 1   | A     | 1870 | C    |
| 1   | A     | 1872 | A    |
| 1   | A     | 1878 | G    |
| 1   | A     | 1882 | C    |
| 1   | A     | 1888 | G    |
| 1   | A     | 1889 | A    |
| 1   | A     | 1906 | G    |
| 1   | A     | 1913 | A    |
| 1   | A     | 1929 | G    |
| 1   | A     | 1930 | G    |
| 1   | A     | 1931 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1937 | A    |
| 1   | A     | 1938 | A    |
| 1   | A     | 1939 | U    |
| 1   | A     | 1955 | U    |
| 1   | A     | 1963 | U    |
| 1   | A     | 1964 | G    |
| 1   | A     | 1967 | C    |
| 1   | A     | 1969 | A    |
| 1   | A     | 1970 | A    |
| 1   | A     | 1971 | A    |
| 1   | A     | 1972 | A    |
| 1   | A     | 1981 | A    |
| 1   | A     | 1982 | C    |
| 1   | A     | 1991 | U    |
| 1   | A     | 1992 | G    |
| 1   | A     | 1993 | U    |
| 1   | A     | 2023 | G    |
| 1   | A     | 2031 | A    |
| 1   | A     | 2032 | G    |
| 1   | A     | 2033 | A    |
| 1   | A     | 2043 | C    |
| 1   | A     | 2055 | C    |
| 1   | A     | 2056 | G    |
| 1   | A     | 2059 | A    |
| 1   | A     | 2060 | A    |
| 1   | A     | 2061 | G    |
| 1   | A     | 2062 | A    |
| 1   | A     | 2069 | G    |
| 1   | A     | 2093 | G    |
| 1   | A     | 2099 | U    |
| 1   | A     | 2100 | G    |
| 1   | A     | 2107 | C    |
| 1   | A     | 2111 | C    |
| 1   | A     | 2113 | U    |
| 1   | A     | 2114 | A    |
| 1   | A     | 2115 | G    |
| 1   | A     | 2116 | G    |
| 1   | A     | 2117 | A    |
| 1   | A     | 2126 | A    |
| 1   | A     | 2127 | G    |
| 1   | A     | 2128 | C    |
| 1   | A     | 2131 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 2132 | U    |
| 1   | A     | 2133 | G    |
| 1   | A     | 2135 | A    |
| 1   | A     | 2136 | C    |
| 1   | A     | 2146 | C    |
| 1   | A     | 2148 | G    |
| 1   | A     | 2157 | G    |
| 1   | A     | 2158 | A    |
| 1   | A     | 2166 | G    |
| 1   | A     | 2168 | G    |
| 1   | A     | 2169 | A    |
| 1   | A     | 2173 | A    |
| 1   | A     | 2176 | A    |
| 1   | A     | 2190 | G    |
| 1   | A     | 2192 | G    |
| 1   | A     | 2198 | A    |
| 1   | A     | 2199 | A    |
| 1   | A     | 2210 | G    |
| 1   | A     | 2211 | G    |
| 1   | A     | 2212 | A    |
| 1   | A     | 2213 | U    |
| 1   | A     | 2215 | G    |
| 1   | A     | 2225 | A    |
| 1   | A     | 2238 | G    |
| 1   | A     | 2239 | G    |
| 1   | A     | 2243 | U    |
| 1   | A     | 2245 | U    |
| 1   | A     | 2275 | C    |
| 1   | A     | 2283 | C    |
| 1   | A     | 2287 | A    |
| 1   | A     | 2307 | G    |
| 1   | A     | 2308 | G    |
| 1   | A     | 2311 | A    |
| 1   | A     | 2312 | U    |
| 1   | A     | 2319 | G    |
| 1   | A     | 2320 | A    |
| 1   | A     | 2325 | G    |
| 1   | A     | 2327 | A    |
| 1   | A     | 2334 | G    |
| 1   | A     | 2336 | A    |
| 1   | A     | 2345 | G    |
| 1   | A     | 2346 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 2347 | C    |
| 1   | A     | 2350 | C    |
| 1   | A     | 2354 | G    |
| 1   | A     | 2379 | G    |
| 1   | A     | 2383 | G    |
| 1   | A     | 2385 | C    |
| 1   | A     | 2391 | G    |
| 1   | A     | 2392 | A    |
| 1   | A     | 2394 | C    |
| 1   | A     | 2402 | C    |
| 1   | A     | 2403 | C    |
| 1   | A     | 2406 | U    |
| 1   | A     | 2410 | G    |
| 1   | A     | 2423 | U    |
| 1   | A     | 2424 | C    |
| 1   | A     | 2425 | A    |
| 1   | A     | 2429 | G    |
| 1   | A     | 2430 | A    |
| 1   | A     | 2435 | A    |
| 1   | A     | 2439 | A    |
| 1   | A     | 2440 | C    |
| 1   | A     | 2441 | C    |
| 1   | A     | 2445 | G    |
| 1   | A     | 2448 | A    |
| 1   | A     | 2469 | A    |
| 1   | A     | 2470 | G    |
| 1   | A     | 2474 | C    |
| 1   | A     | 2475 | C    |
| 1   | A     | 2482 | G    |
| 1   | A     | 2494 | G    |
| 1   | A     | 2502 | G    |
| 1   | A     | 2505 | G    |
| 1   | A     | 2519 | U    |
| 1   | A     | 2520 | C    |
| 1   | A     | 2529 | G    |
| 1   | A     | 2542 | A    |
| 1   | A     | 2543 | G    |
| 1   | A     | 2554 | U    |
| 1   | A     | 2567 | G    |
| 1   | A     | 2569 | G    |
| 1   | A     | 2582 | G    |
| 1   | A     | 2602 | A    |

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| Mol | Chain | Res     | Type |
|-----|-------|---------|------|
| 1   | A     | 2609    | U    |
| 1   | A     | 2611    | U    |
| 1   | A     | 2612    | C    |
| 1   | A     | 2614    | A    |
| 1   | A     | 2623    | G    |
| 1   | A     | 2629    | A    |
| 1   | A     | 2641    | G    |
| 1   | A     | 2646    | C    |
| 1   | A     | 2655    | G    |
| 1   | A     | 2665    | A    |
| 1   | A     | 2673    | G    |
| 1   | A     | 2682    | U    |
| 1   | A     | 2689    | U    |
| 1   | A     | 2690    | C    |
| 1   | A     | 2691    | C    |
| 1   | A     | 2702    | U    |
| 1   | A     | 2703    | C    |
| 1   | A     | 2707    | G    |
| 1   | A     | 2712    | U    |
| 1   | A     | 2712(A) | A    |
| 1   | A     | 2713    | A    |
| 1   | A     | 2714    | G    |
| 1   | A     | 2726    | U    |
| 1   | A     | 2732    | G    |
| 1   | A     | 2733    | A    |
| 1   | A     | 2734    | A    |
| 1   | A     | 2748    | A    |
| 1   | A     | 2752    | C    |
| 1   | A     | 2758    | A    |
| 1   | A     | 2761    | G    |
| 1   | A     | 2764    | A    |
| 1   | A     | 2765    | A    |
| 1   | A     | 2766    | G    |
| 1   | A     | 2777    | G    |
| 1   | A     | 2778    | A    |
| 1   | A     | 2779    | U    |
| 1   | A     | 2780    | G    |
| 1   | A     | 2789    | C    |
| 1   | A     | 2790    | A    |
| 1   | A     | 2791    | C    |
| 1   | A     | 2797    | U    |
| 1   | A     | 2807    | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 2812 | G    |
| 1   | A     | 2818 | G    |
| 1   | A     | 2820 | A    |
| 1   | A     | 2821 | A    |
| 1   | A     | 2833 | G    |
| 1   | A     | 2834 | G    |
| 1   | A     | 2835 | A    |
| 1   | A     | 2867 | G    |
| 1   | A     | 2868 | A    |
| 1   | A     | 2872 | G    |
| 1   | A     | 2879 | C    |
| 1   | A     | 2880 | C    |
| 1   | A     | 2891 | G    |
| 1   | A     | 2892 | A    |
| 1   | A     | 2894 | G    |
| 2   | B     | 8    | U    |
| 2   | B     | 9    | G    |
| 2   | B     | 13   | A    |
| 2   | B     | 15   | A    |
| 2   | B     | 16   | G    |
| 2   | B     | 19   | G    |
| 2   | B     | 22   | U    |
| 2   | B     | 25   | A    |
| 2   | B     | 26   | A    |
| 2   | B     | 27   | C    |
| 2   | B     | 32   | C    |
| 2   | B     | 42   | C    |
| 2   | B     | 45   | A    |
| 2   | B     | 47   | C    |
| 2   | B     | 56   | G    |
| 2   | B     | 67   | G    |
| 2   | B     | 73   | A    |
| 2   | B     | 81   | G    |
| 2   | B     | 89   | G    |
| 2   | B     | 105  | G    |
| 2   | B     | 109  | G    |

All (58) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 27  | G    |
| 1   | A     | 74  | A    |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | A     | 99     | U    |
| 1   | A     | 102    | G    |
| 1   | A     | 195    | A    |
| 1   | A     | 205    | G    |
| 1   | A     | 221    | A    |
| 1   | A     | 222    | A    |
| 1   | A     | 227    | A    |
| 1   | A     | 229    | A    |
| 1   | A     | 242    | G    |
| 1   | A     | 271(B) | G    |
| 1   | A     | 271(C) | U    |
| 1   | A     | 345    | A    |
| 1   | A     | 372    | G    |
| 1   | A     | 404    | C    |
| 1   | A     | 503    | A    |
| 1   | A     | 512    | G    |
| 1   | A     | 587    | C    |
| 1   | A     | 637    | A    |
| 1   | A     | 846    | C    |
| 1   | A     | 856    | C    |
| 1   | A     | 859    | G    |
| 1   | A     | 974(A) | C    |
| 1   | A     | 1012   | U    |
| 1   | A     | 1022   | G    |
| 1   | A     | 1026   | U    |
| 1   | A     | 1045   | A    |
| 1   | A     | 1078   | U    |
| 1   | A     | 1085   | A    |
| 1   | A     | 1130   | U    |
| 1   | A     | 1178   | C    |
| 1   | A     | 1204   | A    |
| 1   | A     | 1210   | A    |
| 1   | A     | 1312   | U    |
| 1   | A     | 1427   | A    |
| 1   | A     | 1558   | A    |
| 1   | A     | 1653   | G    |
| 1   | A     | 1694   | C    |
| 1   | A     | 1799   | G    |
| 1   | A     | 1819   | A    |
| 1   | A     | 1930   | G    |
| 1   | A     | 1980   | G    |
| 1   | A     | 1992   | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 2060 | A    |
| 1   | A     | 2126 | A    |
| 1   | A     | 2405 | G    |
| 1   | A     | 2439 | A    |
| 1   | A     | 2481 | G    |
| 1   | A     | 2518 | A    |
| 1   | A     | 2566 | A    |
| 1   | A     | 2610 | C    |
| 1   | A     | 2689 | U    |
| 1   | A     | 2712 | U    |
| 1   | A     | 2776 | A    |
| 1   | A     | 2832 | U    |
| 1   | A     | 2867 | G    |
| 2   | B     | 66   | A    |

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 257 ligands modelled in this entry, 257 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.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.