



## wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:31 PM BST

PDB ID : 4V19  
EMDB ID: : EMD-2787  
Title : Structure of the large subunit of the mammalian mitoribosome, part 1 of 2  
Authors : Greber, B.J.; Boehringer, D.; Leibundgut, M.; Bieri, P.; Leitner, A.; Schmitz, N.; Aebersold, R.; Ban, N.  
Deposited on : 2014-09-25  
Resolution : 3.40 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.  
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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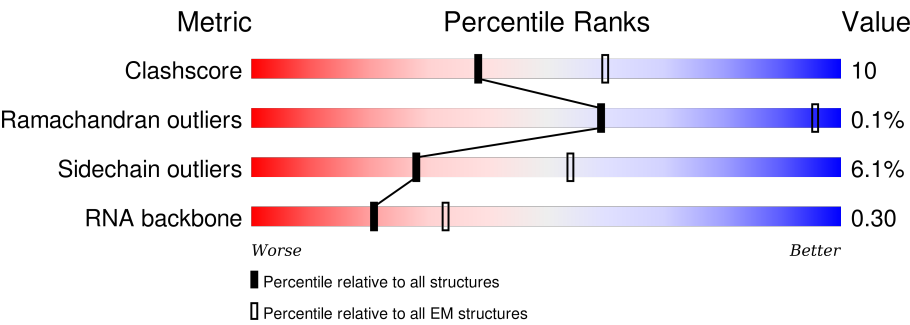
MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk27241

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 3.40 Å.

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






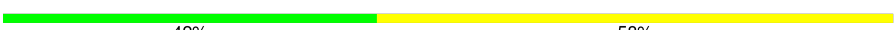
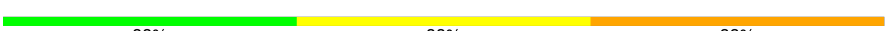







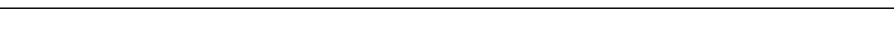
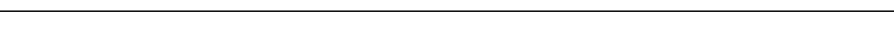
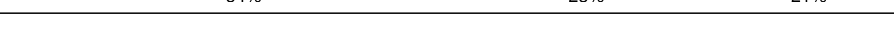









| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) |
|-----------------------|-----------------------------|-----------------------------|
| Clashscore            | 114402                      | 924                         |
| Ramachandran outliers | 111179                      | 726                         |
| Sidechain outliers    | 111093                      | 686                         |
| RNA backbone          | 3027                        | 244                         |

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$

| Mol | Chain | Length | Quality of chain  |
|-----|-------|--------|---|
| 1   | 0     | 148    | <div><div>56%</div><div>20%</div><div>•</div><div>23%</div></div> |
| 2   | 1     | 256    | <div><div>73%</div><div>21%</div><div>•</div><div>5%</div></div>  |
| 3   | 2     | 252    | <div><div>58%</div><div>13%</div><div></div><div>29%</div></div>  |
| 4   | 3     | 161    | <div><div>57%</div><div>16%</div><div>•</div><div>27%</div></div> |
| 5   | 4     | 126    | <div><div>21%</div><div>14%</div><div></div><div>64%</div></div>  |
| 6   | 5     | 188    | <div><div>43%</div><div>15%</div><div></div><div>41%</div></div>  |
| 7   | 6     | 65     | <div><div>35%</div><div>35%</div><div>•</div><div>26%</div></div> |
| 8   | 7     | 95     | <div><div>36%</div><div>9%</div><div>•</div><div>52%</div></div>  |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 9   | 8     | 188    |    |
| 10  | 9     | 100    |    |
| 11  | A     | 1570   |    |
| 12  | B     | 62     |    |
| 13  | C     | 3      |    |
| 13  | Z     | 3      |    |
| 14  | D     | 306    |    |
| 15  | E     | 348    |    |
| 16  | F     | 294    |    |
| 17  | I     | 268    |    |
| 18  | J     | 262    |    |
| 19  | K     | 192    |    |
| 20  | N     | 178    |  |
| 21  | O     | 145    |  |
| 22  | P     | 296    |  |
| 23  | Q     | 251    |  |
| 24  | R     | 169    |  |
| 25  | S     | 180    |  |
| 26  | T     | 292    |  |
| 27  | U     | 149    |  |
| 28  | V     | 209    |  |
| 29  | W     | 210    |  |
| 30  | X     | 150    |  |
| 31  | Y     | 216    |  |

## 2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 69409 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called MITORIBOSOMAL PROTEIN BL27M, MRPL27.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 1   | 0     | 114      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 878   | 564 | 160 | 151 | 3 |         |       |

- Molecule 2 is a protein called MITORIBOSOMAL PROTEIN BL28M, MRPL28.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 2   | 1     | 244      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2036  | 1315 | 363 | 353 | 5 |         |       |

- Molecule 3 is a protein called MITORIBOSOMAL PROTEIN UL29M, MRPL47.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 3   | 2     | 178      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1544  | 990 | 289 | 259 | 6 |         |       |

- Molecule 4 is a protein called MITORIBOSOMAL PROTEIN UL30M, MRPL30.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 4   | 3     | 118      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 968   | 622 | 178 | 165 | 3 |         |       |

- Molecule 5 is a protein called MITORIBOSOMAL PROTEIN BL31M, MRPL55.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 5   | 4     | 45       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 381   | 239 | 77 | 62 | 3 |         |       |

- Molecule 6 is a protein called MITORIBOSOMAL PROTEIN BL32M, MRPL32.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 6   | 5     | 110      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 902   | 553 | 181 | 162 | 6 |         |       |

- Molecule 7 is a protein called MITORIBOSOMAL PROTEIN BL33M, MRPL33.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 7   | 6     | 48       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 391   | 253 | 70 | 66 | 2 |         |       |

- Molecule 8 is a protein called MITORIBOSOMAL PROTEIN BL34M, MRPL34.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 8   | 7     | 46       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 387   | 239 | 89 | 58 | 1 |         |       |

- Molecule 9 is a protein called MITORIBOSOMAL PROTEIN BL35M, MRPL35.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 9   | 8     | 95       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 833   | 539 | 163 | 129 | 2 |         |       |

- Molecule 10 is a protein called MITORIBOSOMAL PROTEIN BL36M, MRPL36.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 10  | 9     | 38       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 335   | 214 | 70 | 47 | 4 |         |       |

- Molecule 11 is a RNA chain called MITORIBOSOMAL 16S RRNA.

| Mol | Chain | Residues | Atoms |       |      |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|-------|
| 11  | A     | 1515     | Total | C     | N    | O     | P    | 0       | 0     |
|     |       |          | 32233 | 14473 | 5860 | 10385 | 1515 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment   | Reference  |
|-------|---------|----------|--------|-----------|------------|
| A     | 127A    | G        | -      | INSERTION | GB 4220565 |

- Molecule 12 is a RNA chain called MITORIBOSOMAL CP TRNA.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 12  | B     | 62       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1225  | 594 | 196 | 373 | 62 |         |       |

- Molecule 13 is a RNA chain called TRNA.

| Mol | Chain | Residues | Atoms |    |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|-------|
| 13  | C     | 3        | Total | C  | N  | O  | P | 0       | 0     |
|     |       |          | 62    | 28 | 11 | 20 | 3 |         |       |
| 13  | Z     | 3        | Total | C  | N  | O  | P | 0       | 0     |
|     |       |          | 62    | 28 | 11 | 20 | 3 |         |       |

- Molecule 14 is a protein called MITORIBOSOMAL PROTEIN UL2M, MRPL2.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 14  | D     | 240      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1860  | 1160 | 371 | 319 | 10 |         |       |

- Molecule 15 is a protein called MITORIBOSOMAL PROTEIN UL3M, MRPL3.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 15  | E     | 307      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2420  | 1554 | 426 | 430 | 10 |         |       |

- Molecule 16 is a protein called MITORIBOSOMAL PROTEIN UL4M, MRPL4.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 16  | F     | 250      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2011  | 1294 | 367 | 344 | 6 |         |       |

- Molecule 17 is a protein called MITORIBOSOMAL PROTEIN BL9M, MRPL9.

| Mol | Chain | Residues | Atoms |     |     |     |  | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 17  | I     | 98       | Total | C   | N   | O   |  | 0       | 0     |
|     |       |          | 805   | 509 | 155 | 141 |  |         |       |

- Molecule 18 is a protein called MITORIBOSOMAL PROTEIN UL10M, MRPL10.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 18  | J     | 168      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1361  | 879 | 248 | 226 | 8 |         |       |

- Molecule 19 is a protein called MITORIBOSOMAL PROTEIN UL11M, MRPL11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19  | K     | 142      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1081  | 690 | 197 | 192 | 2 |         |       |

- Molecule 20 is a protein called MITORIBOSOMAL PROTEIN UL13M, MRPL13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 20  | N     | 177      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1444  | 926 | 258 | 253 | 7 |         |       |

- Molecule 21 is a protein called MITORIBOSOMAL PROTEIN UL14M, MRPL14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 21  | O     | 115      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 896   | 562 | 176 | 154 | 4 |         |       |

- Molecule 22 is a protein called MITORIBOSOMAL PROTEIN UL15M, MRPL15.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 22  | P     | 288      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2312  | 1473 | 430 | 403 | 6 |         |       |

- Molecule 23 is a protein called MITORIBOSOMAL PROTEIN UL16M, MRPL16.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 23  | Q     | 221      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1792  | 1147 | 330 | 305 | 10 |         |       |

- Molecule 24 is a protein called MITORIBOSOMAL PROTEIN BL17M, MRPL17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 24  | R     | 153      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1240  | 777 | 236 | 222 | 5 |         |       |

- Molecule 25 is a protein called MITORIBOSOMAL PROTEIN UL18M, MRPL18.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 25  | S     | 143      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1168  | 733 | 227 | 204 | 4 |         |       |

- Molecule 26 is a protein called MITORIBOSOMAL PROTEIN BL19M, MRPL19.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 26  | T     | 224      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1860  | 1189 | 324 | 338 | 9 |         |       |

- Molecule 27 is a protein called MITORIBOSOMAL PROTEIN BL20M, MRPL20.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 27  | U     | 140      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1159  | 732 | 239 | 185 | 3 |         |       |

- Molecule 28 is a protein called MITORIBOSOMAL PROTEIN BL21M, MRPL21.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 28  | V     | 155      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1231  | 789 | 219 | 219 | 4 |         |       |

- Molecule 29 is a protein called MITORIBOSOMAL PROTEIN UL22M, MRPL22.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 29  | W     | 166      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1374  | 876 | 258 | 234 | 6 |         |       |

- Molecule 30 is a protein called MITORIBOSOMAL PROTEIN UL23M, MRPL23.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 30  | X     | 134      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1120  | 715 | 217 | 186 | 2 |         |       |

- Molecule 31 is a protein called MITORIBOSOMAL PROTEIN UL24M, MRPL24.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 31  | Y     | 204      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1663  | 1047 | 305 | 306 | 5 |         |       |

- Molecule 32 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 32  | 9     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 32  | 5     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |

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

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 33  | P     | 2        | Total | Mg | 0       |
|     |       |          | 2     | 2  |         |
| 33  | Q     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |

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| Mol | Chain | Residues | Atoms        |           | AltConf |
|-----|-------|----------|--------------|-----------|---------|
| 33  | A     | 163      | Total<br>163 | Mg<br>163 | 0       |
| 33  | D     | 2        | Total<br>2   | Mg<br>2   | 0       |
| 33  | R     | 1        | Total<br>1   | Mg<br>1   | 0       |

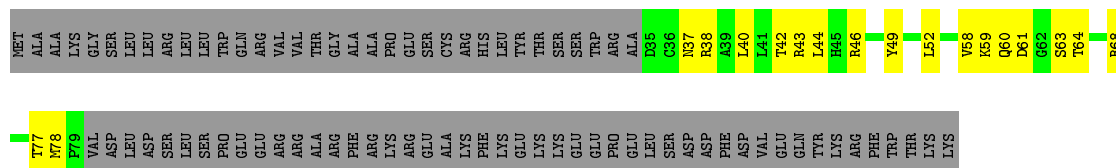
- Molecule 34 is water.

| Mol | Chain | Residues | Atoms        |          | AltConf |
|-----|-------|----------|--------------|----------|---------|
| 34  | A     | 192      | Total<br>192 | O<br>192 | 0       |
| 34  | D     | 6        | Total<br>6   | O<br>6   | 0       |
| 34  | P     | 6        | Total<br>6   | O<br>6   | 0       |

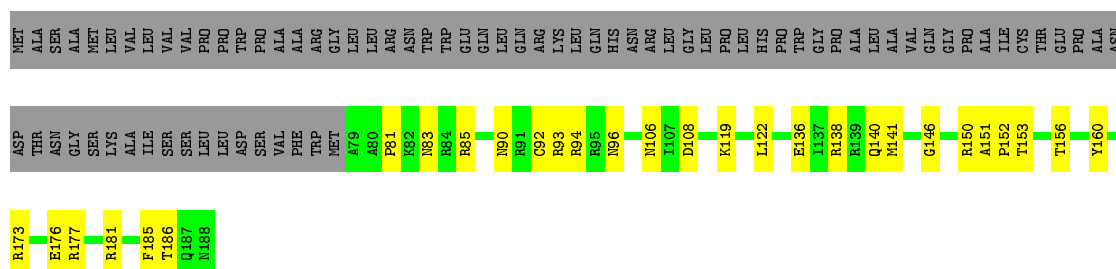




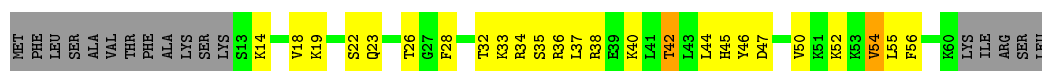
- Molecule 5: MITORIBOSOMAL PROTEIN BL31M, MRPL55



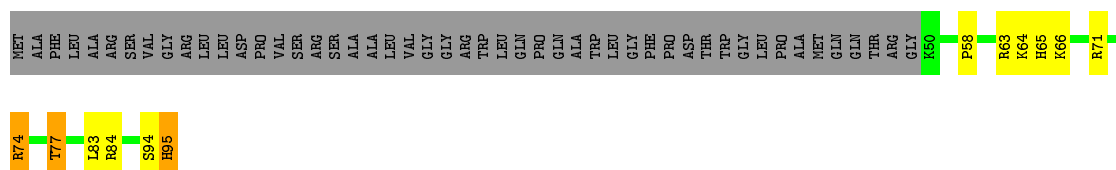
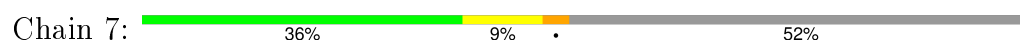
- Molecule 6: MITORIBOSOMAL PROTEIN BL32M, MRPL32



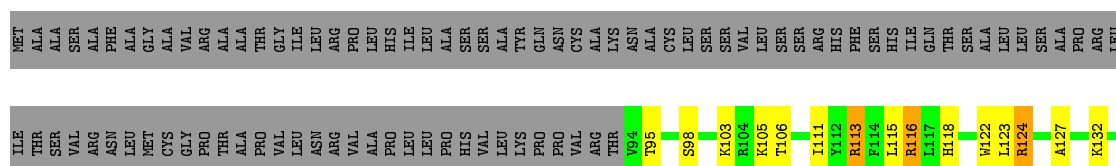
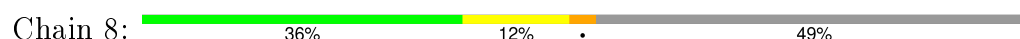
- Molecule 7: MITORIBOSOMAL PROTEIN BL33M, MRPL33

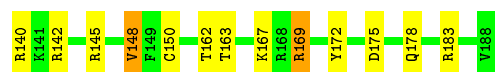


- Molecule 8: MITORIBOSOMAL PROTEIN BL34M, MRPL34



- Molecule 9: MITORIBOSOMAL PROTEIN BL35M, MRPL35

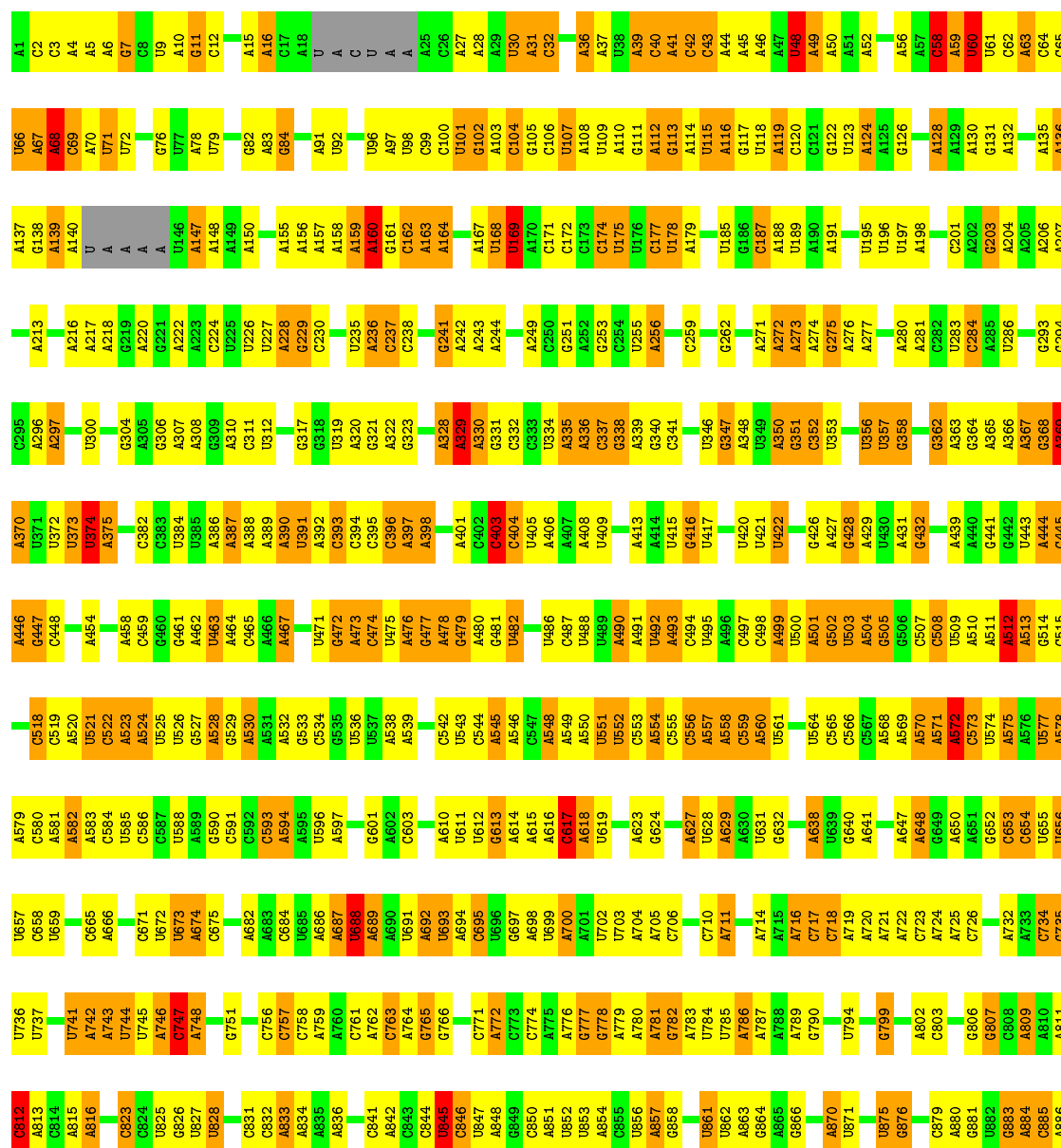




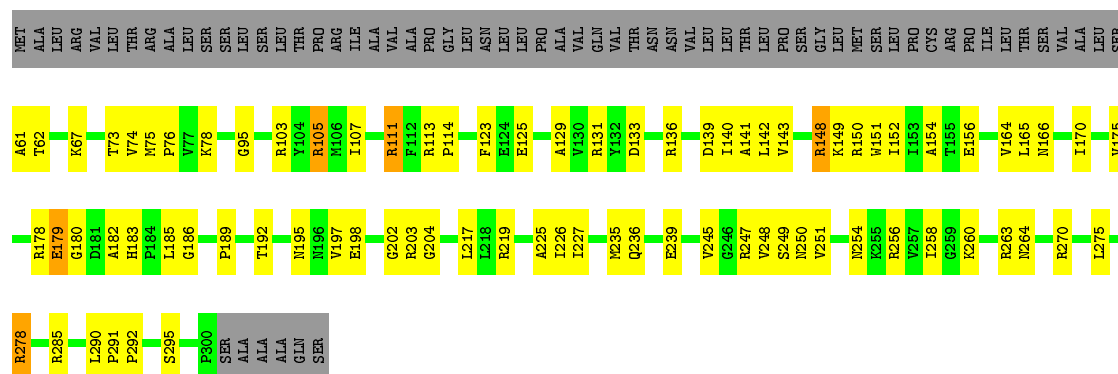
• Molecule 10: MITORIBOSOMAL PROTEIN BL36M, MRPL36



• Molecule 11: MITORIBOSOMAL 16S RRNA

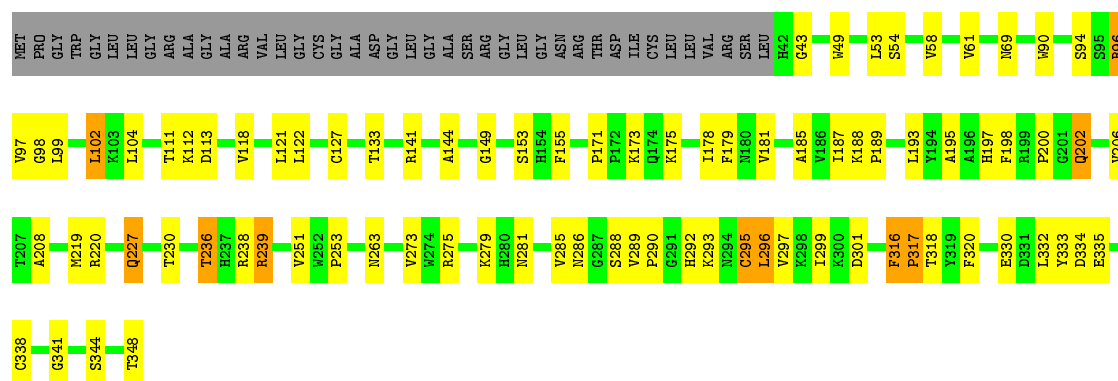






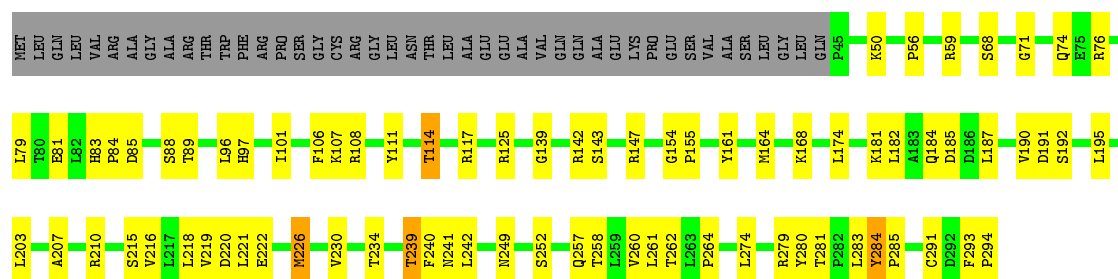
• Molecule 15: MITORIBOSOMAL PROTEIN UL3M, MRPL3

Chain E: 64% 22% 12%



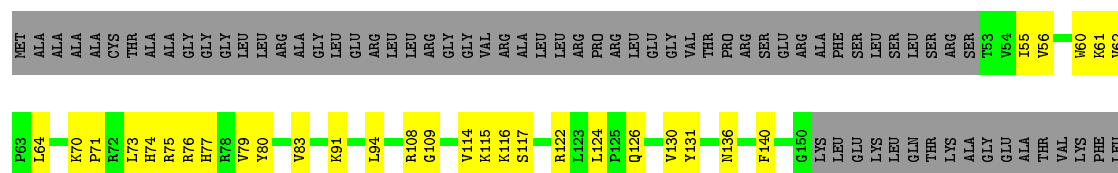
• Molecule 16: MITORIBOSOMAL PROTEIN UL4M, MRPL4

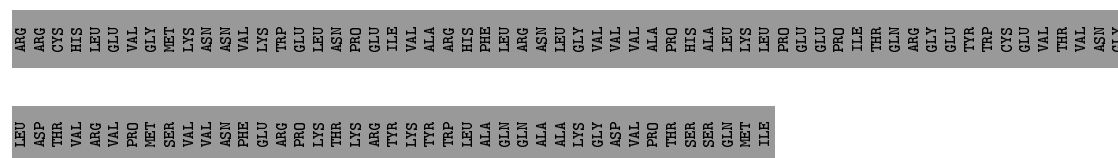
Chain F: 59% 25% 15%



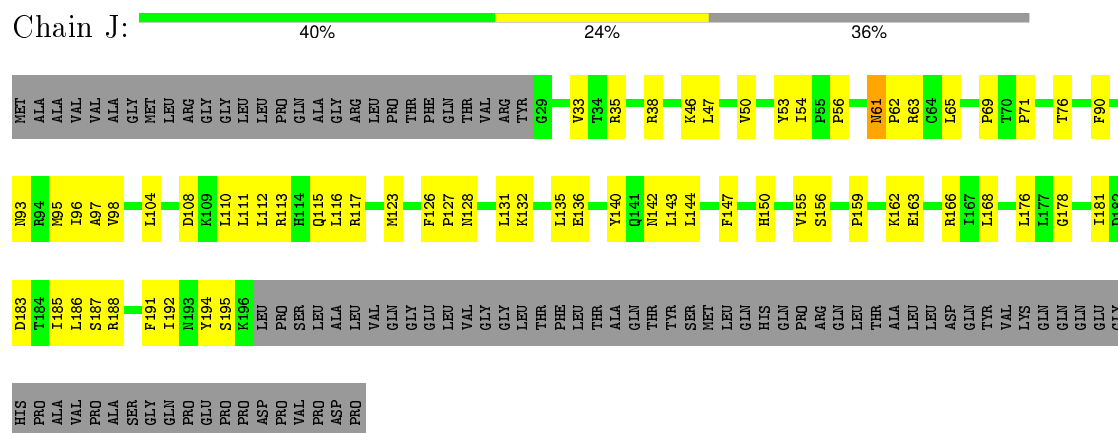
• Molecule 17: MITORIBOSOMAL PROTEIN BL9M, MRPL9

Chain I: 25% 12% 63%

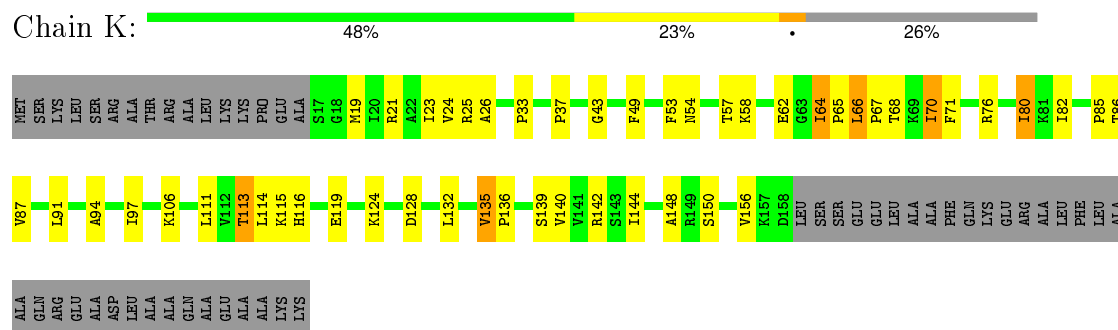




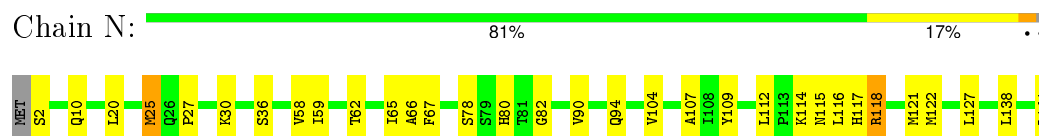
• Molecule 18: MITORIBOSOMAL PROTEIN UL10M, MRPL10



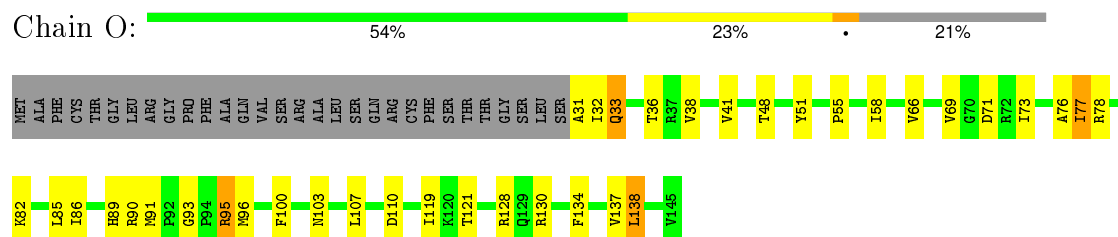
• Molecule 19: MITORIBOSOMAL PROTEIN UL11M, MRPL11




• Molecule 20: MITORIBOSOMAL PROTEIN UL13M, MRPL13

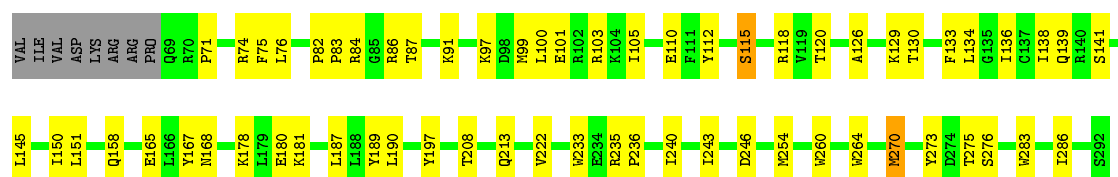


• Molecule 21: MITORIBOSOMAL PROTEIN UL14M, MRPL14



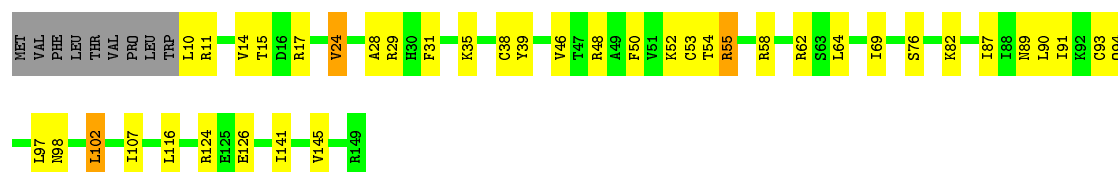
• Molecule 22: MITORIBOSOMAL PROTEIN UL15M, MRPL15

Chain T: 



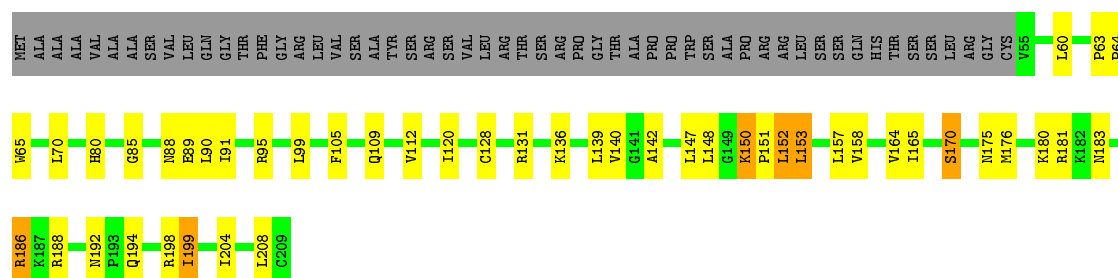
- Molecule 27: MITORIBOSOMAL PROTEIN BL20M, MRPL20

Chain U: 67% 25% 6%



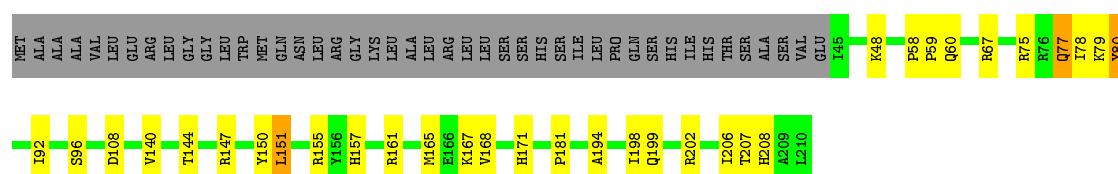
- Molecule 28: MITORIBOSOMAL PROTEIN BL21M, MRPL21

Chain V: 52% 20% 26%



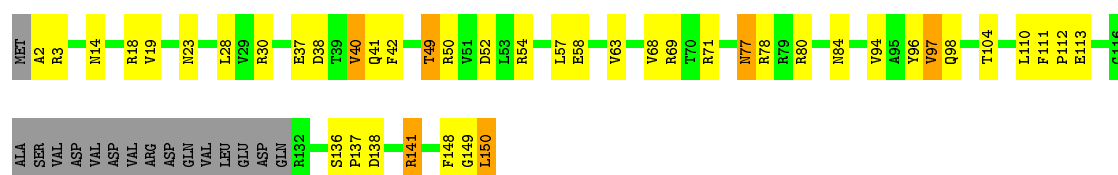
- Molecule 29: MITORIBOSOMAL PROTEIN UL22M, MRPL22

Chain W: 63% 14% 21%

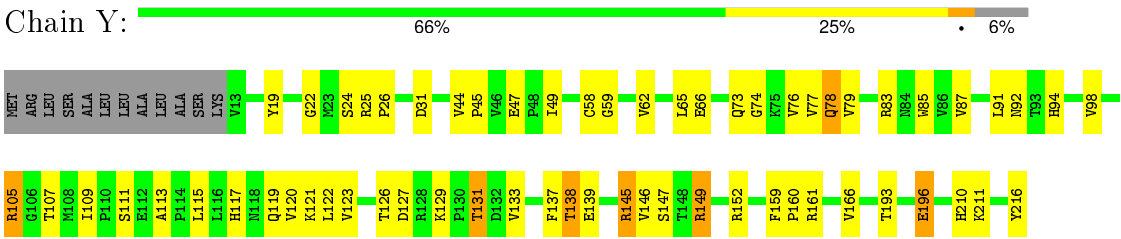


- Molecule 30: MITORIBOSOMAL PROTEIN UL23M, MRPL23

Chain X: 61% 25% 11%



- Molecule 31: MITORIBOSOMAL PROTEIN UL24M, MRPL24



## 4 Experimental information

| Property                             | Value               | Source    |
|--------------------------------------|---------------------|-----------|
| Reconstruction method                | SINGLE PARTICLE     | Depositor |
| Imposed symmetry                     | POINT, Not provided | Depositor |
| Number of images                     | Not provided        | Depositor |
| Resolution determination method      | Not provided        | Depositor |
| CTF correction method                | PER DETECTOR FRAME  | Depositor |
| Microscope                           | FEI TITAN KRIOS     | Depositor |
| Voltage (kV)                         | 300                 | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 2000                | Depositor |
| Minimum defocus (nm)                 | 800                 | Depositor |
| Maximum defocus (nm)                 | 3000                | Depositor |
| Magnification                        | 59000               | Depositor |
| Image detector                       | FEI FALCON II       | Depositor |

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: Y5P, ZN, P5P, 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         | $\# Z  > 2$    | RMSZ        | $\# Z  > 2$      |
| 1   | 0     | 0.43         | 0/901          | 0.59        | 0/1217           |
| 10  | 9     | 0.47         | 0/342          | 0.57        | 0/450            |
| 11  | A     | 0.62         | 2/36094 (0.0%) | 1.06        | 72/56186 (0.1%)  |
| 13  | C     | 0.50         | 0/68           | 1.01        | 0/103            |
| 13  | Z     | 0.32         | 0/68           | 0.86        | 0/103            |
| 14  | D     | 0.38         | 0/1898         | 0.58        | 0/2555           |
| 15  | E     | 0.38         | 0/2493         | 0.61        | 0/3387           |
| 16  | F     | 0.42         | 0/2069         | 0.58        | 0/2816           |
| 17  | I     | 0.35         | 0/819          | 0.52        | 0/1101           |
| 18  | J     | 0.35         | 0/1392         | 0.55        | 0/1881           |
| 19  | K     | 0.35         | 0/1099         | 0.49        | 0/1480           |
| 2   | 1     | 0.35         | 0/2093         | 0.51        | 0/2835           |
| 20  | N     | 0.40         | 0/1487         | 0.57        | 0/2017           |
| 21  | O     | 0.36         | 0/912          | 0.56        | 0/1231           |
| 22  | P     | 0.40         | 0/2368         | 0.60        | 0/3198           |
| 23  | Q     | 0.39         | 0/1838         | 0.57        | 0/2475           |
| 24  | R     | 0.39         | 0/1262         | 0.57        | 0/1700           |
| 25  | S     | 0.36         | 0/1197         | 0.55        | 0/1624           |
| 26  | T     | 0.35         | 0/1903         | 0.54        | 0/2567           |
| 27  | U     | 0.46         | 0/1179         | 0.61        | 0/1578           |
| 28  | V     | 0.40         | 0/1256         | 0.58        | 0/1706           |
| 29  | W     | 0.42         | 0/1407         | 0.57        | 0/1891           |
| 3   | 2     | 0.36         | 0/1582         | 0.52        | 0/2118           |
| 30  | X     | 0.37         | 0/1149         | 0.59        | 0/1554           |
| 31  | Y     | 0.35         | 0/1704         | 0.54        | 0/2310           |
| 4   | 3     | 0.41         | 0/993          | 0.59        | 0/1341           |
| 5   | 4     | 0.29         | 0/388          | 0.57        | 0/523            |
| 6   | 5     | 0.38         | 0/917          | 0.53        | 0/1227           |
| 7   | 6     | 0.35         | 0/396          | 0.54        | 0/526            |
| 8   | 7     | 0.45         | 0/395          | 0.55        | 0/524            |
| 9   | 8     | 0.48         | 0/853          | 0.60        | 0/1136           |
| All | All   | 0.52         | 2/72522 (0.0%) | 0.87        | 72/105360 (0.1%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 15  | E     | 0                   | 2                   |
| 28  | V     | 0                   | 1                   |
| All | All   | 0                   | 3                   |

All (2) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 11  | A     | 1255 | A    | N9-C4 | -6.05 | 1.34        | 1.37     |
| 11  | A     | 490  | A    | C8-N7 | 5.63  | 1.35        | 1.31     |

All (72) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 11  | A     | 374  | U    | N1-C2-O2   | 8.42  | 128.70      | 122.80   |
| 11  | A     | 374  | U    | N3-C2-O2   | -8.24 | 116.43      | 122.20   |
| 11  | A     | 48   | U    | N3-C2-O2   | -7.50 | 116.95      | 122.20   |
| 11  | A     | 593  | C    | C6-N1-C2   | -7.38 | 117.35      | 120.30   |
| 11  | A     | 1413 | G    | C4-N9-C1'  | 7.14  | 135.78      | 126.50   |
| 11  | A     | 490  | A    | C2-N3-C4   | 7.01  | 114.11      | 110.60   |
| 11  | A     | 353  | U    | O5'-P-OP1  | -6.83 | 99.55       | 105.70   |
| 11  | A     | 104  | C    | C2-N1-C1'  | 6.64  | 126.10      | 118.80   |
| 11  | A     | 845  | U    | C5-C6-N1   | 6.43  | 125.92      | 122.70   |
| 11  | A     | 559  | C    | N1-C2-O2   | 6.43  | 122.76      | 118.90   |
| 11  | A     | 104  | C    | N1-C2-O2   | 6.42  | 122.75      | 118.90   |
| 11  | A     | 1255 | A    | C5-N7-C8   | -6.39 | 100.70      | 103.90   |
| 11  | A     | 169  | U    | N3-C2-O2   | -6.37 | 117.74      | 122.20   |
| 11  | A     | 1433 | C    | C2-N1-C1'  | 6.35  | 125.79      | 118.80   |
| 11  | A     | 237  | C    | O4'-C1'-N1 | 6.34  | 113.27      | 108.20   |
| 11  | A     | 284  | C    | C6-N1-C2   | -6.30 | 117.78      | 120.30   |
| 11  | A     | 518  | C    | C2-N1-C1'  | 6.17  | 125.59      | 118.80   |
| 11  | A     | 812  | C    | N1-C2-O2   | 6.15  | 122.59      | 118.90   |
| 11  | A     | 572  | A    | C2-N3-C4   | 6.08  | 113.64      | 110.60   |
| 11  | A     | 374  | U    | C2-N1-C1'  | 6.05  | 124.97      | 117.70   |
| 11  | A     | 1205 | C    | C6-N1-C2   | -6.03 | 117.89      | 120.30   |
| 11  | A     | 60   | U    | N3-C2-O2   | -6.01 | 117.99      | 122.20   |
| 11  | A     | 160  | A    | P-O3'-C3'  | 6.00  | 126.91      | 119.70   |
| 11  | A     | 931  | A    | P-O3'-C3'  | 5.97  | 126.86      | 119.70   |
| 11  | A     | 512  | A    | P-O3'-C3'  | 5.91  | 126.79      | 119.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 11  | A     | 1413 | G    | N3-C4-C5   | -5.90 | 125.65      | 128.60   |
| 11  | A     | 1433 | C    | C6-N1-C2   | -5.88 | 117.95      | 120.30   |
| 11  | A     | 329  | A    | C8-N9-C4   | -5.85 | 103.46      | 105.80   |
| 11  | A     | 474  | C    | C6-N1-C2   | -5.85 | 117.96      | 120.30   |
| 11  | A     | 369  | A    | C8-N9-C4   | -5.82 | 103.47      | 105.80   |
| 11  | A     | 48   | U    | N1-C2-O2   | 5.81  | 126.87      | 122.80   |
| 11  | A     | 58   | C    | N3-C2-O2   | -5.80 | 117.84      | 121.90   |
| 11  | A     | 1413 | G    | N3-C4-N9   | 5.79  | 129.47      | 126.00   |
| 11  | A     | 688  | U    | C2-N1-C1'  | 5.78  | 124.63      | 117.70   |
| 11  | A     | 373  | U    | N1-C2-O2   | 5.77  | 126.84      | 122.80   |
| 11  | A     | 1140 | U    | P-O3'-C3'  | 5.73  | 126.58      | 119.70   |
| 11  | A     | 898  | G    | C4-N9-C1'  | 5.71  | 133.92      | 126.50   |
| 11  | A     | 1255 | A    | C4-C5-N7   | 5.66  | 113.53      | 110.70   |
| 11  | A     | 1413 | G    | C8-N9-C1'  | -5.65 | 119.65      | 127.00   |
| 11  | A     | 881  | G    | C4-N9-C1'  | 5.63  | 133.83      | 126.50   |
| 11  | A     | 931  | A    | OP1-P-O3'  | 5.58  | 117.48      | 105.20   |
| 11  | A     | 104  | C    | C5-C6-N1   | 5.57  | 123.78      | 121.00   |
| 11  | A     | 68   | A    | O4'-C1'-N9 | 5.55  | 112.64      | 108.20   |
| 11  | A     | 823  | C    | C2-N1-C1'  | 5.55  | 124.90      | 118.80   |
| 11  | A     | 1139 | A    | C8-N9-C4   | -5.53 | 103.59      | 105.80   |
| 11  | A     | 1229 | U    | C5-C6-N1   | 5.52  | 125.46      | 122.70   |
| 11  | A     | 373  | U    | C2-N1-C1'  | 5.50  | 124.30      | 117.70   |
| 11  | A     | 58   | C    | N1-C2-O2   | 5.48  | 122.19      | 118.90   |
| 11  | A     | 823  | C    | N3-C2-O2   | -5.42 | 118.11      | 121.90   |
| 11  | A     | 799  | G    | C4-N9-C1'  | -5.41 | 119.47      | 126.50   |
| 11  | A     | 593  | C    | N3-C2-O2   | -5.39 | 118.13      | 121.90   |
| 11  | A     | 1013 | C    | P-O3'-C3'  | 5.36  | 126.14      | 119.70   |
| 11  | A     | 823  | C    | N1-C2-O2   | 5.36  | 122.12      | 118.90   |
| 11  | A     | 174  | C    | C2-N1-C1'  | 5.36  | 124.69      | 118.80   |
| 11  | A     | 1568 | C    | N1-C2-O2   | 5.35  | 122.11      | 118.90   |
| 11  | A     | 174  | C    | C6-N1-C2   | -5.34 | 118.16      | 120.30   |
| 11  | A     | 66   | U    | C2-N1-C1'  | 5.34  | 124.11      | 117.70   |
| 11  | A     | 1166 | A    | P-O3'-C3'  | 5.31  | 126.08      | 119.70   |
| 11  | A     | 1518 | U    | P-O3'-C3'  | 5.30  | 126.07      | 119.70   |
| 11  | A     | 617  | C    | P-O3'-C3'  | 5.30  | 126.06      | 119.70   |
| 11  | A     | 765  | G    | P-O3'-C3'  | 5.30  | 126.06      | 119.70   |
| 11  | A     | 467  | A    | O4'-C1'-N9 | 5.26  | 112.41      | 108.20   |
| 11  | A     | 559  | C    | N3-C2-O2   | -5.25 | 118.23      | 121.90   |
| 11  | A     | 201  | C    | C2-N1-C1'  | -5.22 | 113.06      | 118.80   |
| 11  | A     | 1234 | C    | C5-C6-N1   | 5.18  | 123.59      | 121.00   |
| 11  | A     | 593  | C    | C2-N1-C1'  | 5.15  | 124.47      | 118.80   |
| 11  | A     | 747  | C    | O4'-C1'-N1 | 5.07  | 112.26      | 108.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 11  | A     | 1523 | C    | N1-C2-O2    | 5.07  | 121.94      | 118.90   |
| 11  | A     | 572  | A    | C3'-C2'-C1' | 5.05  | 105.54      | 101.50   |
| 11  | A     | 403  | C    | C2-N1-C1'   | 5.03  | 124.33      | 118.80   |
| 11  | A     | 812  | C    | N3-C2-O2    | -5.01 | 118.39      | 121.90   |
| 11  | A     | 306  | G    | P-O3'-C3'   | 5.00  | 125.71      | 119.70   |

There are no chirality outliers.

All (3) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 15  | E     | 316 | PHE  | Peptide |
| 15  | E     | 43  | GLY  | Peptide |
| 28  | V     | 150 | LYS  | Peptide |

## 5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | 0     | 878   | 0        | 896      | 20      | 0            |
| 2   | 1     | 2036  | 0        | 2058     | 36      | 0            |
| 3   | 2     | 1544  | 0        | 1580     | 26      | 0            |
| 4   | 3     | 968   | 0        | 1018     | 23      | 0            |
| 5   | 4     | 381   | 0        | 400      | 9       | 0            |
| 6   | 5     | 902   | 0        | 916      | 22      | 0            |
| 7   | 6     | 391   | 0        | 429      | 18      | 0            |
| 8   | 7     | 387   | 0        | 413      | 10      | 0            |
| 9   | 8     | 833   | 0        | 883      | 17      | 0            |
| 10  | 9     | 335   | 0        | 359      | 11      | 0            |
| 11  | A     | 32233 | 0        | 16310    | 440     | 0            |
| 12  | B     | 1225  | 0        | 675      | 29      | 0            |
| 13  | C     | 62    | 0        | 34       | 1       | 0            |
| 13  | Z     | 62    | 0        | 34       | 0       | 0            |
| 14  | D     | 1860  | 0        | 1923     | 58      | 0            |
| 15  | E     | 2420  | 0        | 2418     | 63      | 0            |
| 16  | F     | 2011  | 0        | 2049     | 50      | 0            |
| 17  | I     | 805   | 0        | 845      | 21      | 0            |
| 18  | J     | 1361  | 0        | 1449     | 46      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 19  | K     | 1081  | 0        | 1146     | 36      | 0            |
| 20  | N     | 1444  | 0        | 1437     | 22      | 0            |
| 21  | O     | 896   | 0        | 946      | 25      | 0            |
| 22  | P     | 2312  | 0        | 2373     | 63      | 0            |
| 23  | Q     | 1792  | 0        | 1832     | 31      | 0            |
| 24  | R     | 1240  | 0        | 1260     | 40      | 0            |
| 25  | S     | 1168  | 0        | 1159     | 46      | 0            |
| 26  | T     | 1860  | 0        | 1875     | 45      | 0            |
| 27  | U     | 1159  | 0        | 1228     | 35      | 0            |
| 28  | V     | 1231  | 0        | 1278     | 35      | 0            |
| 29  | W     | 1374  | 0        | 1405     | 20      | 0            |
| 30  | X     | 1120  | 0        | 1133     | 27      | 0            |
| 31  | Y     | 1663  | 0        | 1665     | 50      | 0            |
| 32  | 5     | 1     | 0        | 0        | 0       | 0            |
| 32  | 9     | 1     | 0        | 0        | 0       | 0            |
| 33  | A     | 163   | 0        | 0        | 0       | 0            |
| 33  | D     | 2     | 0        | 0        | 0       | 0            |
| 33  | P     | 2     | 0        | 0        | 0       | 0            |
| 33  | Q     | 1     | 0        | 0        | 0       | 0            |
| 33  | R     | 1     | 0        | 0        | 0       | 0            |
| 34  | A     | 192   | 0        | 0        | 5       | 0            |
| 34  | D     | 6     | 0        | 0        | 0       | 0            |
| 34  | P     | 6     | 0        | 0        | 4       | 0            |
| All | All   | 69409 | 0        | 53426    | 1171    | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (1171) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:A:346:U:H4'    | 11:A:347:G:H5'    | 1.53                     | 0.91              |
| 27:U:54:THR:HG21  | 28:V:176:MET:H    | 1.38                     | 0.88              |
| 14:D:111:ARG:HH11 | 14:D:182:ALA:HB2  | 1.40                     | 0.86              |
| 16:F:262:THR:HG22 | 16:F:264:PRO:HD2  | 1.59                     | 0.85              |
| 18:J:156:SER:HB3  | 18:J:159:PRO:HB3  | 1.59                     | 0.84              |
| 22:P:137:GLY:HA3  | 22:P:157:GLN:HG3  | 1.60                     | 0.84              |
| 31:Y:122:LEU:HD23 | 31:Y:133:VAL:HG21 | 1.61                     | 0.83              |
| 2:1:96:LYS:O      | 11:A:60:U:O2'     | 1.98                     | 0.82              |
| 11:A:1230:G:O2'   | 11:A:1246:C:N4    | 2.13                     | 0.81              |
| 11:A:68:A:O2'     | 11:A:69:C:O4'     | 1.97                     | 0.81              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:D:186:GLY:HA3  | 14:D:239:GLU:HG3  | 1.63                     | 0.81              |
| 11:A:845:U:H5'    | 11:A:845:U:H6     | 1.46                     | 0.80              |
| 5:4:61:ASP:HB3    | 5:4:63:SER:H      | 1.46                     | 0.79              |
| 11:A:177:C:H1'    | 27:U:55:ARG:HH22  | 1.47                     | 0.79              |
| 15:E:206:VAL:HG22 | 15:E:299:ILE:HD13 | 1.64                     | 0.79              |
| 25:S:86:THR:HG22  | 25:S:88:HIS:H     | 1.47                     | 0.79              |
| 31:Y:127:ASP:H    | 31:Y:152:ARG:HH12 | 1.29                     | 0.77              |
| 3:2:182:LYS:NZ    | 11:A:28:A:OP2     | 2.16                     | 0.77              |
| 19:K:70:ILE:HG12  | 19:K:80:ILE:HD12  | 1.67                     | 0.76              |
| 11:A:136:A:OP2    | 31:Y:83:ARG:NH2   | 2.18                     | 0.76              |
| 11:A:512:A:H4'    | 11:A:513:A:H5''   | 1.65                     | 0.76              |
| 1:0:56:MET:H      | 1:0:59:HIS:HD2    | 1.32                     | 0.76              |
| 11:A:993:C:H5''   | 24:R:13:ARG:HH22  | 1.49                     | 0.76              |
| 8:7:74:ARG:NH2    | 11:A:31:A:O2'     | 2.19                     | 0.75              |
| 11:A:746:A:O2'    | 11:A:747:C:O5'    | 2.04                     | 0.75              |
| 11:A:893:U:OP1    | 14:D:285:ARG:NH2  | 2.20                     | 0.75              |
| 11:A:572:A:N3     | 11:A:572:A:H2'    | 2.02                     | 0.75              |
| 18:J:142:ASN:HB2  | 18:J:185:ILE:HG21 | 1.70                     | 0.73              |
| 11:A:163:A:OP2    | 27:U:52:LYS:NZ    | 2.21                     | 0.73              |
| 30:X:40:VAL:HG23  | 30:X:97:VAL:HG23  | 1.70                     | 0.73              |
| 9:8:142:ARG:NH1   | 11:A:1191:C:OP2   | 2.20                     | 0.73              |
| 11:A:786:A:H3'    | 24:R:10:SER:HB2   | 1.71                     | 0.73              |
| 11:A:1250:G:N3    | 22:P:77:ARG:NH2   | 2.37                     | 0.73              |
| 11:A:1312:U:H5'   | 11:A:1391:C:H5''  | 1.69                     | 0.73              |
| 3:2:175:PHE:O     | 3:2:214:ARG:NH2   | 2.22                     | 0.72              |
| 3:2:120:GLU:HG2   | 30:X:110:LEU:HD12 | 1.70                     | 0.72              |
| 25:S:85:ARG:HB3   | 25:S:120:ARG:HH12 | 1.55                     | 0.72              |
| 15:E:317:PRO:HG2  | 15:E:320:PHE:HE1  | 1.54                     | 0.71              |
| 14:D:195:ASN:HD22 | 14:D:248:VAL:HG22 | 1.53                     | 0.71              |
| 22:P:97:SER:HB2   | 22:P:143:GLU:HB2  | 1.72                     | 0.71              |
| 22:P:94:GLN:OE1   | 34:P:5543:HOH:O   | 2.08                     | 0.71              |
| 4:3:126:GLN:HE22  | 4:3:146:VAL:HG13  | 1.55                     | 0.71              |
| 16:F:85:ASP:HB3   | 16:F:274:LEU:HD21 | 1.73                     | 0.71              |
| 31:Y:105:ARG:HD3  | 31:Y:105:ARG:H    | 1.55                     | 0.71              |
| 7:6:47:ASP:HB2    | 7:6:54:VAL:HG21   | 1.72                     | 0.71              |
| 11:A:947:A:N3     | 11:A:1372:U:H5''  | 2.06                     | 0.70              |
| 11:A:1440:U:H5''  | 15:E:253:PRO:HA   | 1.73                     | 0.70              |
| 19:K:43:GLY:HA3   | 19:K:76:ARG:HH11  | 1.56                     | 0.70              |
| 18:J:93:ASN:HB2   | 18:J:96:ILE:HG12  | 1.74                     | 0.70              |
| 15:E:96:ARG:NH2   | 15:E:197:HIS:O    | 2.21                     | 0.70              |
| 11:A:1184:U:O2'   | 11:A:1185:U:O4'   | 2.10                     | 0.70              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:P:205:LEU:HG   | 22:P:263:ARG:HH21 | 1.56                     | 0.70              |
| 15:E:181:VAL:HG13 | 15:E:185:ALA:HB3  | 1.73                     | 0.70              |
| 11:A:370:A:O2'    | 22:P:71:GLN:NE2   | 2.26                     | 0.69              |
| 22:P:104:LEU:HD11 | 22:P:126:GLY:HA3  | 1.74                     | 0.69              |
| 5:4:52:LEU:HG     | 5:4:68:ARG:HB3    | 1.75                     | 0.69              |
| 11:A:1048:C:H2'   | 11:A:1325:U:H4'   | 1.74                     | 0.69              |
| 24:R:43:GLU:HB2   | 24:R:123:VAL:HG23 | 1.74                     | 0.69              |
| 11:A:462:A:H3'    | 11:A:463:U:H5'    | 1.75                     | 0.69              |
| 11:A:69:C:O2'     | 11:A:70:A:O5'     | 2.08                     | 0.69              |
| 11:A:747:C:O2'    | 11:A:748:A:H5''   | 1.92                     | 0.69              |
| 23:Q:131:ILE:HB   | 23:Q:149:HIS:HB3  | 1.75                     | 0.69              |
| 30:X:49:THR:HG23  | 30:X:52:ASP:HB2   | 1.76                     | 0.68              |
| 4:3:75:THR:HG22   | 4:3:86:ILE:HD13   | 1.73                     | 0.68              |
| 25:S:126:GLU:HG2  | 25:S:160:ARG:HB3  | 1.74                     | 0.68              |
| 11:A:9:U:O4       | 11:A:107:U:O2'    | 2.11                     | 0.68              |
| 15:E:187:ILE:HG22 | 15:E:188:LYS:H    | 1.58                     | 0.68              |
| 6:5:140:GLN:NE2   | 6:5:176:GLU:O     | 2.23                     | 0.68              |
| 25:S:39:VAL:HG12  | 25:S:41:ASN:H     | 1.59                     | 0.68              |
| 11:A:185:U:O4'    | 11:A:432:G:O2'    | 2.12                     | 0.68              |
| 25:S:116:LEU:HG   | 25:S:117:TYR:H    | 1.58                     | 0.68              |
| 31:Y:129:LYS:HD3  | 31:Y:149:ARG:HH21 | 1.59                     | 0.68              |
| 11:A:403:C:H2'    | 11:A:404:C:H5'    | 1.77                     | 0.67              |
| 30:X:68:VAL:HG22  | 30:X:97:VAL:HG12  | 1.77                     | 0.67              |
| 15:E:227:GLN:HG3  | 15:E:236:THR:O    | 1.93                     | 0.67              |
| 16:F:226:MET:HE1  | 16:F:242:LEU:HD11 | 1.74                     | 0.67              |
| 21:O:128:ARG:HA   | 21:O:138:LEU:HD21 | 1.76                     | 0.67              |
| 8:7:63:ARG:HH21   | 8:7:64:LYS:HE2    | 1.59                     | 0.67              |
| 22:P:186:ILE:HD13 | 22:P:201:PRO:HG3  | 1.77                     | 0.67              |
| 2:1:16:LEU:HD12   | 2:1:21:TYR:HB3    | 1.77                     | 0.67              |
| 5:4:59:LYS:HA     | 5:4:78:MET:HB2    | 1.77                     | 0.67              |
| 11:A:504:A:OP1    | 19:K:21:ARG:NH1   | 2.28                     | 0.67              |
| 11:A:794:U:H4'    | 26:T:260:TRP:HZ3  | 1.59                     | 0.66              |
| 2:1:156:LYS:NZ    | 2:1:205:GLY:O     | 2.28                     | 0.66              |
| 5:4:37:ASN:HD22   | 5:4:40:LEU:HD12   | 1.59                     | 0.66              |
| 26:T:165:GLU:HB2  | 26:T:168:ASN:HB2  | 1.77                     | 0.66              |
| 11:A:1148:G:OP2   | 11:A:1173:C:O2'   | 2.07                     | 0.66              |
| 11:A:428:G:OP1    | 22:P:62:ARG:NH2   | 2.29                     | 0.66              |
| 11:A:1344:A:HO2'  | 11:A:1534:U:HO2'  | 1.43                     | 0.66              |
| 22:P:264:GLN:NE2  | 22:P:269:LEU:O    | 2.29                     | 0.66              |
| 14:D:219:ARG:HE   | 14:D:226:ILE:HD12 | 1.61                     | 0.65              |
| 31:Y:131:THR:HG21 | 31:Y:147:SER:HB3  | 1.78                     | 0.65              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:8:172:TYR:HB2   | 9:8:175:ASP:HB2   | 1.77                     | 0.65              |
| 4:3:74:SER:HB2    | 11:A:471:U:H5''   | 1.78                     | 0.65              |
| 11:A:931:A:O2'    | 11:A:932:U:OP1    | 2.14                     | 0.65              |
| 18:J:33:VAL:HB    | 23:Q:69:LEU:HB3   | 1.78                     | 0.65              |
| 11:A:1454:C:H2'   | 11:A:1455:A:H2'   | 1.78                     | 0.65              |
| 11:A:111:G:H2'    | 11:A:112:A:H5''   | 1.78                     | 0.65              |
| 24:R:38:ARG:HG2   | 24:R:39:HIS:CD2   | 2.31                     | 0.64              |
| 18:J:186:LEU:HD13 | 18:J:194:TYR:CE2  | 2.33                     | 0.64              |
| 23:Q:118:MET:HB3  | 23:Q:163:MET:HE1  | 1.80                     | 0.64              |
| 16:F:257:GLN:HB3  | 22:P:21:ARG:HH11  | 1.62                     | 0.64              |
| 31:Y:19:TYR:OH    | 31:Y:31:ASP:OD2   | 2.16                     | 0.64              |
| 29:W:77:GLN:H     | 29:W:171:HIS:CD2  | 2.16                     | 0.64              |
| 29:W:77:GLN:H     | 29:W:171:HIS:HD2  | 1.45                     | 0.64              |
| 12:B:9:P5P:H5'2   | 12:B:47:P5P:H1'   | 1.79                     | 0.64              |
| 21:O:130:ARG:HD2  | 21:O:134:PHE:HE2  | 1.63                     | 0.64              |
| 16:F:283:LEU:HB2  | 22:P:125:ARG:HH12 | 1.63                     | 0.64              |
| 11:A:476:A:O2'    | 28:V:192:ASN:ND2  | 2.30                     | 0.64              |
| 11:A:1550:C:H5'   | 11:A:1551:A:OP1   | 1.97                     | 0.64              |
| 11:A:1510:U:H2'   | 11:A:1511:U:H5''  | 1.79                     | 0.64              |
| 11:A:1209:A:P     | 25:S:176:ARG:HH22 | 2.20                     | 0.64              |
| 9:8:116:ARG:HG3   | 9:8:122:TRP:CE2   | 2.33                     | 0.64              |
| 11:A:228:A:H4'    | 11:A:229:G:H5'    | 1.80                     | 0.63              |
| 14:D:236:GLN:HB3  | 14:D:295:SER:HA   | 1.80                     | 0.63              |
| 18:J:104:LEU:HB3  | 18:J:108:ASP:HB2  | 1.79                     | 0.63              |
| 11:A:178:U:O2'    | 11:A:188:A:O4'    | 2.14                     | 0.63              |
| 15:E:341:GLY:HA2  | 26:T:105:ILE:HD11 | 1.80                     | 0.63              |
| 11:A:1512:A:H2'   | 11:A:1513:A:H5''  | 1.81                     | 0.63              |
| 23:Q:81:GLU:O     | 23:Q:123:ARG:NH2  | 2.31                     | 0.63              |
| 19:K:57:THR:HG23  | 19:K:66:LEU:HD21  | 1.80                     | 0.63              |
| 14:D:107:ILE:HD11 | 14:D:140:ILE:HD13 | 1.81                     | 0.63              |
| 11:A:785:U:OP1    | 24:R:16:ARG:NH1   | 2.32                     | 0.63              |
| 3:2:189:PRO:HA    | 31:Y:216:TYR:OH   | 1.99                     | 0.63              |
| 3:2:89:CYS:HB3    | 3:2:93:ARG:HE     | 1.64                     | 0.63              |
| 11:A:572:A:O2'    | 11:A:573:C:O2     | 2.17                     | 0.62              |
| 19:K:19:MET:HG2   | 19:K:71:PHE:HD1   | 1.64                     | 0.62              |
| 11:A:391:U:H2'    | 11:A:392:A:C8     | 2.34                     | 0.62              |
| 25:S:174:GLU:HG3  | 25:S:175:PRO:HD2  | 1.80                     | 0.62              |
| 18:J:54:ILE:HD12  | 23:Q:211:ASN:HB3  | 1.79                     | 0.62              |
| 4:3:36:PHE:CE1    | 23:Q:228:LYS:HA   | 2.33                     | 0.62              |
| 19:K:94:ALA:HB1   | 19:K:116:HIS:HD2  | 1.63                     | 0.62              |
| 16:F:220:ASP:OD1  | 16:F:221:LEU:N    | 2.32                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:P:116:ILE:HD12 | 22:P:152:VAL:HG13 | 1.81                     | 0.62              |
| 21:O:32:ILE:HD11  | 21:O:38:VAL:HG12  | 1.82                     | 0.62              |
| 16:F:83:HIS:HD2   | 16:F:85:ASP:H     | 1.47                     | 0.62              |
| 11:A:1343:A:H4'   | 11:A:1449:U:OP1   | 2.00                     | 0.62              |
| 11:A:335:A:H4'    | 11:A:336:A:OP2    | 2.00                     | 0.62              |
| 14:D:123:PHE:HB2  | 14:D:166:ASN:HB2  | 1.81                     | 0.62              |
| 11:A:1546:A:H5'   | 11:A:1547:A:OP1   | 2.00                     | 0.62              |
| 11:A:911:G:H21    | 11:A:912:A:N6     | 1.97                     | 0.62              |
| 11:A:809:A:H1'    | 15:E:230:THR:HG23 | 1.83                     | 0.61              |
| 14:D:198:GLU:OE2  | 14:D:202:GLY:N    | 2.33                     | 0.61              |
| 31:Y:133:VAL:HG13 | 31:Y:145:ARG:HB3  | 1.82                     | 0.61              |
| 6:5:90:ASN:OD1    | 6:5:93:ARG:NH2    | 2.33                     | 0.61              |
| 27:U:97:LEU:HA    | 28:V:109:GLN:HE22 | 1.64                     | 0.61              |
| 24:R:110:ILE:HD11 | 24:R:123:VAL:HB   | 1.81                     | 0.61              |
| 17:I:94:LEU:HB3   | 17:I:114:VAL:HG23 | 1.82                     | 0.61              |
| 11:A:747:C:O2     | 30:X:54:ARG:NH1   | 2.30                     | 0.61              |
| 11:A:163:A:HO2'   | 11:A:1014:C:H5    | 1.49                     | 0.61              |
| 11:A:330:A:O2'    | 11:A:338:G:N7     | 2.33                     | 0.61              |
| 26:T:74:ARG:HB3   | 26:T:283:TRP:CZ2  | 2.35                     | 0.61              |
| 10:9:93:PRO:HG2   | 11:A:1349:U:OP1   | 2.00                     | 0.61              |
| 12:B:23:P5P:OP2   | 25:S:113:LYS:NZ   | 2.32                     | 0.61              |
| 16:F:56:PRO:HG2   | 16:F:59:ARG:HB3   | 1.81                     | 0.61              |
| 1:0:61:VAL:HG21   | 1:0:97:VAL:HG23   | 1.81                     | 0.61              |
| 11:A:220:A:N7     | 16:F:281:THR:OG1  | 2.34                     | 0.61              |
| 6:5:136:GLU:HG2   | 6:5:177:ARG:NH2   | 2.14                     | 0.61              |
| 11:A:875:U:O2'    | 11:A:876:G:OP2    | 2.17                     | 0.60              |
| 5:4:44:LEU:HD22   | 5:4:49:TYR:CG     | 2.36                     | 0.60              |
| 3:2:126:LEU:HD12  | 3:2:127:PRO:HD2   | 1.83                     | 0.60              |
| 2:1:177:HIS:CD2   | 2:1:183:ARG:HD2   | 2.36                     | 0.60              |
| 15:E:285:VAL:HG12 | 15:E:286:ASN:H    | 1.65                     | 0.60              |
| 14:D:179:GLU:HA   | 14:D:245:VAL:O    | 2.00                     | 0.60              |
| 11:A:68:A:O2'     | 11:A:69:C:O5'     | 2.18                     | 0.60              |
| 18:J:56:PRO:HA    | 23:Q:210:GLN:HE21 | 1.66                     | 0.60              |
| 24:R:129:ASN:HD22 | 24:R:131:LEU:HD12 | 1.66                     | 0.60              |
| 16:F:74:GLN:O     | 16:F:210:ARG:NH2  | 2.35                     | 0.60              |
| 1:0:76:HIS:HD2    | 25:S:70:THR:HG21  | 1.67                     | 0.60              |
| 21:O:110:ASP:N    | 21:O:110:ASP:OD1  | 2.34                     | 0.60              |
| 31:Y:131:THR:HG23 | 31:Y:149:ARG:HB3  | 1.84                     | 0.60              |
| 11:A:895:A:H2'    | 11:A:896:C:H6     | 1.67                     | 0.60              |
| 22:P:54:LYS:N     | 22:P:58:GLN:OE1   | 2.31                     | 0.60              |
| 11:A:627:A:O2'    | 11:A:629:A:OP1    | 2.20                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:A:58:C:H2'     | 11:A:59:A:H5''    | 1.85                     | 0.59              |
| 18:J:163:GLU:HG3  | 18:J:166:ARG:CZ   | 2.31                     | 0.59              |
| 1:0:56:MET:H      | 1:0:59:HIS:CD2    | 2.19                     | 0.59              |
| 30:X:37:GLU:HB3   | 30:X:104:THR:HG23 | 1.84                     | 0.59              |
| 11:A:503:U:H4'    | 11:A:504:A:H5'    | 1.85                     | 0.59              |
| 18:J:110:LEU:HB3  | 19:K:132:LEU:HD13 | 1.85                     | 0.59              |
| 18:J:111:LEU:O    | 18:J:115:GLN:HG2  | 2.01                     | 0.59              |
| 11:A:689:A:OP2    | 34:A:5366:HOH:O   | 2.16                     | 0.59              |
| 26:T:120:THR:HG23 | 26:T:130:THR:HG23 | 1.83                     | 0.59              |
| 11:A:816:A:OP1    | 11:A:816:A:H4'    | 2.00                     | 0.59              |
| 11:A:1408:A:H5'   | 11:A:1409:G:OP2   | 2.01                     | 0.59              |
| 11:A:404:C:H2'    | 11:A:405:U:O4'    | 2.01                     | 0.59              |
| 25:S:54:ARG:NH2   | 25:S:141:ILE:HG22 | 2.18                     | 0.59              |
| 18:J:128:ASN:ND2  | 18:J:147:PHE:O    | 2.28                     | 0.59              |
| 12:B:60:Y5P:H4A   | 12:B:61:Y5P:H4    | 1.85                     | 0.59              |
| 19:K:26:ALA:HA    | 19:K:57:THR:HG22  | 1.84                     | 0.59              |
| 18:J:98:VAL:N     | 18:J:178:GLY:O    | 2.35                     | 0.59              |
| 30:X:50:ARG:NH1   | 30:X:69:ARG:HA    | 2.18                     | 0.59              |
| 18:J:95:MET:HB3   | 18:J:156:SER:HB2  | 1.83                     | 0.59              |
| 23:Q:50:LEU:H     | 23:Q:110:ASN:HD21 | 1.50                     | 0.59              |
| 11:A:319:U:OP1    | 14:D:61:ALA:N     | 2.35                     | 0.59              |
| 22:P:130:GLN:NE2  | 34:P:5540:HOH:O   | 2.36                     | 0.59              |
| 15:E:98:GLY:HA3   | 15:E:179:PHE:CE1  | 2.38                     | 0.59              |
| 15:E:99:LEU:HD21  | 15:E:193:LEU:HB3  | 1.85                     | 0.58              |
| 24:R:118:ARG:HG2  | 29:W:108:ASP:OD1  | 2.02                     | 0.58              |
| 3:2:123:ARG:NH1   | 30:X:30:ARG:O     | 2.35                     | 0.58              |
| 5:4:58:VAL:HG22   | 5:4:64:THR:HG22   | 1.84                     | 0.58              |
| 12:B:41:P5P:C6    | 12:B:42:Y5P:H4    | 2.32                     | 0.58              |
| 11:A:694:A:H3'    | 11:A:695:C:H5''   | 1.84                     | 0.58              |
| 11:A:744:U:OP2    | 11:A:744:U:H4'    | 2.02                     | 0.58              |
| 11:A:65:C:OP1     | 11:A:67:A:N6      | 2.37                     | 0.58              |
| 11:A:1250:G:N7    | 34:A:5125:HOH:O   | 2.31                     | 0.58              |
| 5:4:44:LEU:HD21   | 5:4:46:ARG:HB2    | 1.86                     | 0.58              |
| 11:A:445:C:H1'    | 11:A:1278:C:O2'   | 2.02                     | 0.58              |
| 20:N:27:PRO:HG2   | 20:N:30:LYS:HB2   | 1.85                     | 0.58              |
| 11:A:163:A:OP1    | 27:U:48:ARG:HD2   | 2.03                     | 0.58              |
| 19:K:87:VAL:HG22  | 19:K:124:LYS:HD3  | 1.85                     | 0.58              |
| 15:E:334:ASP:OD1  | 15:E:335:GLU:N    | 2.37                     | 0.58              |
| 9:8:132:LYS:HE3   | 11:A:1230:G:H3'   | 1.86                     | 0.58              |
| 7:6:34:ARG:HG3    | 7:6:36:ARG:HG2    | 1.86                     | 0.58              |
| 11:A:1228:U:H5'   | 11:A:1229:U:OP2   | 2.03                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:A:958:U:O2'    | 11:A:959:A:OP2    | 2.20                     | 0.57              |
| 16:F:85:ASP:O     | 16:F:89:THR:OG1   | 2.22                     | 0.57              |
| 23:Q:172:VAL:HG12 | 23:Q:176:LEU:HG   | 1.86                     | 0.57              |
| 11:A:1481:C:H5'   | 15:E:290:PRO:HA   | 1.86                     | 0.57              |
| 1:0:74:ARG:HD3    | 1:0:75:TRP:CZ2    | 2.38                     | 0.57              |
| 28:V:186:ARG:HH21 | 28:V:188:ARG:NH2  | 2.02                     | 0.57              |
| 11:A:79:U:O2'     | 17:I:61:LYS:NZ    | 2.36                     | 0.57              |
| 11:A:988:U:H3'    | 11:A:989:C:H2'    | 1.85                     | 0.57              |
| 24:R:32:LEU:HB3   | 24:R:52:LEU:HD22  | 1.86                     | 0.57              |
| 11:A:174:C:H5'    | 20:N:115:ASN:HB3  | 1.85                     | 0.57              |
| 14:D:156:GLU:HA   | 14:D:249:SER:HA   | 1.87                     | 0.57              |
| 30:X:149:GLY:O    | 30:X:150:LEU:HB2  | 2.05                     | 0.57              |
| 22:P:100:ARG:HH21 | 22:P:126:GLY:HA2  | 1.70                     | 0.57              |
| 11:A:884:A:H2'    | 11:A:885:C:O4'    | 2.04                     | 0.57              |
| 16:F:182:LEU:HD13 | 16:F:187:LEU:HD23 | 1.85                     | 0.57              |
| 10:9:92:ASN:HD22  | 10:9:95:HIS:CE1   | 2.23                     | 0.57              |
| 21:O:93:GLY:O     | 21:O:95:ARG:NH1   | 2.38                     | 0.57              |
| 11:A:1002:A:H2'   | 11:A:1003:G:H5''  | 1.87                     | 0.57              |
| 7:6:37:LEU:HD11   | 7:6:40:LYS:HA     | 1.86                     | 0.57              |
| 16:F:226:MET:HE2  | 16:F:242:LEU:HD21 | 1.87                     | 0.57              |
| 3:2:190:TRP:HB3   | 31:Y:216:TYR:CE1  | 2.40                     | 0.57              |
| 11:A:743:A:H5'    | 11:A:744:U:H5''   | 1.85                     | 0.57              |
| 11:A:638:A:OP1    | 29:W:147:ARG:NH1  | 2.38                     | 0.57              |
| 6:5:85:ARG:NH1    | 11:A:640:G:OP1    | 2.38                     | 0.56              |
| 3:2:232:LYS:NZ    | 11:A:10:A:OP1     | 2.36                     | 0.56              |
| 16:F:215:SER:HA   | 16:F:239:THR:HG22 | 1.86                     | 0.56              |
| 6:5:151:ALA:N     | 24:R:84:ASP:OD2   | 2.36                     | 0.56              |
| 11:A:503:U:C2     | 11:A:505:G:H5''   | 2.40                     | 0.56              |
| 16:F:83:HIS:CD2   | 16:F:85:ASP:H     | 2.22                     | 0.56              |
| 22:P:217:ALA:HB2  | 22:P:228:ARG:HB2  | 1.87                     | 0.56              |
| 30:X:2:ALA:HB2    | 30:X:19:VAL:HG11  | 1.87                     | 0.56              |
| 2:1:87:LEU:HD23   | 2:1:104:VAL:HB    | 1.88                     | 0.56              |
| 16:F:249:ASN:ND2  | 16:F:252:SER:H    | 2.03                     | 0.56              |
| 11:A:975:G:H5'    | 11:A:976:G:OP2    | 2.05                     | 0.56              |
| 18:J:168:LEU:HD13 | 18:J:176:LEU:HB2  | 1.88                     | 0.56              |
| 11:A:686:A:H3'    | 11:A:687:A:H4'    | 1.88                     | 0.56              |
| 15:E:122:LEU:HD13 | 15:E:299:ILE:HD11 | 1.86                     | 0.56              |
| 11:A:39:A:H4'     | 11:A:40:C:OP2     | 2.06                     | 0.56              |
| 30:X:71:ARG:NH1   | 30:X:96:TYR:OH    | 2.39                     | 0.56              |
| 1:0:76:HIS:CD2    | 25:S:70:THR:HG21  | 2.41                     | 0.56              |
| 17:I:56:VAL:CG1   | 17:I:80:TYR:HB3   | 2.35                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:F:207:ALA:HB2  | 16:F:240:PHE:HZ   | 1.70                     | 0.56              |
| 24:R:143:LEU:HA   | 24:R:148:GLN:HE21 | 1.69                     | 0.56              |
| 11:A:911:G:H21    | 11:A:912:A:H62    | 1.54                     | 0.56              |
| 16:F:257:GLN:HB3  | 22:P:21:ARG:NH1   | 2.21                     | 0.56              |
| 18:J:97:ALA:HB1   | 18:J:176:LEU:HD11 | 1.88                     | 0.56              |
| 11:A:687:A:N1     | 29:W:155:ARG:HG3  | 2.21                     | 0.56              |
| 19:K:25:ARG:HA    | 19:K:65:PRO:HB3   | 1.87                     | 0.56              |
| 4:3:76:LYS:HZ1    | 11:A:472:G:H8     | 1.54                     | 0.56              |
| 7:6:23:GLN:NE2    | 7:6:55:LEU:HB3    | 2.21                     | 0.56              |
| 11:A:241:G:OP1    | 16:F:117:ARG:NH2  | 2.37                     | 0.55              |
| 11:A:794:U:H4'    | 26:T:260:TRP:CZ3  | 2.40                     | 0.55              |
| 22:P:287:ASP:HB3  | 22:P:290:LEU:HB2  | 1.87                     | 0.55              |
| 18:J:162:LYS:O    | 18:J:166:ARG:HG3  | 2.07                     | 0.55              |
| 11:A:716:A:H5'    | 11:A:717:C:OP2    | 2.06                     | 0.55              |
| 27:U:141:ILE:HG21 | 28:V:80:HIS:CE1   | 2.41                     | 0.55              |
| 20:N:62:THR:O     | 20:N:65:ILE:HG13  | 2.06                     | 0.55              |
| 11:A:551:U:H2'    | 11:A:552:U:H5''   | 1.89                     | 0.55              |
| 6:5:90:ASN:O      | 6:5:94:ARG:HG2    | 2.06                     | 0.55              |
| 11:A:174:C:H5'    | 20:N:115:ASN:CB   | 2.36                     | 0.55              |
| 14:D:76:PRO:HB2   | 14:D:103:ARG:HD3  | 1.88                     | 0.55              |
| 3:2:228:LEU:HD11  | 11:A:11:G:H5''    | 1.88                     | 0.55              |
| 11:A:1002:A:N6    | 34:A:5048:HOH:O   | 2.39                     | 0.55              |
| 11:A:1125:A:H2'   | 11:A:1126:A:C8    | 2.41                     | 0.55              |
| 15:E:200:PRO:HG3  | 15:E:332:LEU:HB3  | 1.87                     | 0.55              |
| 11:A:1074:A:H2'   | 11:A:1075:A:C8    | 2.42                     | 0.55              |
| 11:A:395:C:H5'    | 11:A:396:C:OP1    | 2.06                     | 0.55              |
| 11:A:366:A:O2'    | 11:A:367:A:OP1    | 2.18                     | 0.55              |
| 26:T:246:ASP:OD1  | 26:T:246:ASP:N    | 2.40                     | 0.55              |
| 16:F:219:VAL:HB   | 16:F:261:LEU:HD23 | 1.89                     | 0.55              |
| 16:F:284:TYR:HB2  | 16:F:285:PRO:HD2  | 1.89                     | 0.55              |
| 10:9:65:THR:HG23  | 10:9:100:MET:HB3  | 1.88                     | 0.55              |
| 19:K:140:VAL:O    | 19:K:144:ILE:HG12 | 2.06                     | 0.55              |
| 17:I:122:ARG:O    | 17:I:126:GLN:HG2  | 2.07                     | 0.55              |
| 15:E:53:LEU:HA    | 24:R:147:ASN:HD21 | 1.71                     | 0.55              |
| 14:D:111:ARG:HE   | 14:D:152:ILE:HD12 | 1.71                     | 0.54              |
| 11:A:60:U:C5      | 11:A:61:U:H1'     | 2.41                     | 0.54              |
| 16:F:83:HIS:CG    | 16:F:274:LEU:HD11 | 2.42                     | 0.54              |
| 1:0:76:HIS:HE1    | 1:0:128:LYS:HD2   | 1.72                     | 0.54              |
| 27:U:54:THR:CG2   | 28:V:176:MET:H    | 2.18                     | 0.54              |
| 11:A:979:U:H5'    | 11:A:980:U:OP2    | 2.08                     | 0.54              |
| 11:A:889:A:H3'    | 11:A:890:G:C8     | 2.43                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:A:718:C:H5'    | 14:D:75:MET:HG2   | 1.90                     | 0.54              |
| 11:A:1290:A:H4'   | 23:Q:111:ARG:CZ   | 2.37                     | 0.54              |
| 11:A:428:G:H5'    | 22:P:57:ARG:HD3   | 1.88                     | 0.54              |
| 11:A:78:A:OP1     | 22:P:87:HIS:HE1   | 1.91                     | 0.54              |
| 16:F:249:ASN:HD21 | 16:F:252:SER:H    | 1.55                     | 0.54              |
| 11:A:530:A:N6     | 19:K:150:SER:HB3  | 2.21                     | 0.54              |
| 11:A:368:G:H2'    | 11:A:369:A:H5''   | 1.89                     | 0.54              |
| 31:Y:49:ILE:HD11  | 31:Y:117:HIS:CE1  | 2.42                     | 0.54              |
| 27:U:28:ALA:HA    | 27:U:31:PHE:CE1   | 2.42                     | 0.54              |
| 31:Y:78:GLN:HE21  | 31:Y:87:VAL:HG21  | 1.73                     | 0.54              |
| 11:A:857:A:H5''   | 14:D:67:LYS:HE2   | 1.90                     | 0.54              |
| 2:1:41:VAL:HG11   | 2:1:83:GLU:HB3    | 1.89                     | 0.54              |
| 8:7:95:HIS:CD2    | 11:A:124:A:H5''   | 2.41                     | 0.54              |
| 11:A:446:A:H5'    | 11:A:447:G:OP2    | 2.07                     | 0.54              |
| 19:K:49:PHE:CE1   | 19:K:80:ILE:HD13  | 2.42                     | 0.54              |
| 17:I:109:GLY:HA2  | 17:I:140:PHE:CE2  | 2.43                     | 0.54              |
| 26:T:233:TRP:HB3  | 26:T:240:ILE:HD12 | 1.89                     | 0.54              |
| 11:A:658:C:O3'    | 24:R:81:THR:HG21  | 2.08                     | 0.54              |
| 11:A:1431:U:H4'   | 11:A:1432:U:H5'   | 1.89                     | 0.54              |
| 10:9:85:TRP:CZ2   | 11:A:492:U:O2'    | 2.61                     | 0.54              |
| 14:D:73:THR:HG22  | 14:D:75:MET:H     | 1.72                     | 0.53              |
| 15:E:295:CYS:SG   | 15:E:296:LEU:N    | 2.82                     | 0.53              |
| 11:A:924:U:O2'    | 11:A:925:A:H8     | 1.91                     | 0.53              |
| 2:1:20:ILE:HA     | 2:1:23:ARG:HD2    | 1.90                     | 0.53              |
| 11:A:585:U:H2'    | 11:A:586:C:H6     | 1.71                     | 0.53              |
| 16:F:83:HIS:CD2   | 16:F:274:LEU:HD11 | 2.43                     | 0.53              |
| 11:A:1300:U:OP1   | 11:A:1358:U:O2'   | 2.17                     | 0.53              |
| 11:A:577:U:O2'    | 11:A:578:A:OP1    | 2.20                     | 0.53              |
| 14:D:178:ARG:HG2  | 14:D:179:GLU:H    | 1.73                     | 0.53              |
| 1:0:135:PRO:HB3   | 25:S:63:ARG:NH1   | 2.23                     | 0.53              |
| 22:P:273:TRP:CD1  | 22:P:284:LYS:HB3  | 2.44                     | 0.53              |
| 28:V:99:LEU:HD23  | 28:V:142:ALA:HB2  | 1.90                     | 0.53              |
| 11:A:297:A:C2     | 11:A:335:A:H2'    | 2.42                     | 0.53              |
| 11:A:975:G:N7     | 34:A:5239:HOH:O   | 2.34                     | 0.53              |
| 25:S:66:ARG:HH11  | 25:S:180:GLU:HG2  | 1.73                     | 0.53              |
| 11:A:444:A:H2     | 23:Q:244:LYS:HD2  | 1.74                     | 0.53              |
| 11:A:362:G:H8     | 11:A:362:G:H5'    | 1.72                     | 0.53              |
| 22:P:130:GLN:NE2  | 34:P:5544:HOH:O   | 2.38                     | 0.53              |
| 15:E:133:THR:HB   | 15:E:144:ALA:HB3  | 1.91                     | 0.53              |
| 15:E:104:LEU:HB2  | 15:E:121:LEU:HB2  | 1.90                     | 0.53              |
| 21:O:100:PHE:HB3  | 26:T:158:GLN:HE21 | 1.73                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:P:130:GLN:NE2  | 34:P:5541:HOH:O   | 2.41                     | 0.53              |
| 25:S:89:HIS:CD2   | 25:S:119:THR:HG21 | 2.44                     | 0.53              |
| 11:A:272:A:O2'    | 11:A:273:A:H5''   | 2.09                     | 0.53              |
| 3:2:239:LYS:NZ    | 31:Y:45:PRO:HG3   | 2.23                     | 0.53              |
| 11:A:403:C:C2'    | 11:A:404:C:H5'    | 2.38                     | 0.53              |
| 22:P:199:PRO:HA   | 22:P:274:VAL:HG22 | 1.91                     | 0.53              |
| 16:F:108:ARG:HG2  | 16:F:161:TYR:CD1  | 2.44                     | 0.53              |
| 26:T:110:GLU:OE1  | 26:T:110:GLU:N    | 2.40                     | 0.53              |
| 11:A:69:C:HO2'    | 11:A:70:A:P       | 2.30                     | 0.53              |
| 12:B:59:P5P:C6    | 12:B:60:Y5P:H4    | 2.39                     | 0.53              |
| 25:S:107:THR:HG21 | 25:S:119:THR:HG23 | 1.90                     | 0.53              |
| 24:R:84:ASP:O     | 24:R:87:PRO:HD2   | 2.08                     | 0.53              |
| 11:A:617:C:H4'    | 11:A:618:A:OP1    | 2.09                     | 0.53              |
| 11:A:352:C:OP1    | 11:A:375:A:O2'    | 2.23                     | 0.53              |
| 19:K:62:GLU:HB2   | 19:K:64:ILE:HD11  | 1.91                     | 0.53              |
| 4:3:148:ARG:HH21  | 4:3:151:LEU:HD13  | 1.74                     | 0.53              |
| 18:J:93:ASN:ND2   | 18:J:155:VAL:HG22 | 2.24                     | 0.52              |
| 22:P:196:ARG:HB3  | 22:P:198:GLN:HG3  | 1.91                     | 0.52              |
| 28:V:147:LEU:HD13 | 28:V:157:LEU:HD21 | 1.90                     | 0.52              |
| 4:3:72:ILE:HD11   | 4:3:118:ARG:HD2   | 1.90                     | 0.52              |
| 11:A:653:C:H3'    | 11:A:654:C:C6     | 2.44                     | 0.52              |
| 11:A:1234:C:H6    | 11:A:1234:C:O5'   | 1.93                     | 0.52              |
| 7:6:44:LEU:HA     | 7:6:54:VAL:O      | 2.09                     | 0.52              |
| 14:D:114:PRO:HA   | 14:D:123:PHE:CZ   | 2.44                     | 0.52              |
| 29:W:150:TYR:CE2  | 29:W:168:VAL:HG13 | 2.45                     | 0.52              |
| 18:J:90:PHE:CZ    | 18:J:135:LEU:HD21 | 2.44                     | 0.52              |
| 15:E:202:GLN:NE2  | 15:E:301:ASP:OD1  | 2.41                     | 0.52              |
| 20:N:112:LEU:HD13 | 20:N:121:MET:HG3  | 1.91                     | 0.52              |
| 7:6:33:LYS:HE3    | 7:6:37:LEU:HD13   | 1.91                     | 0.52              |
| 11:A:658:C:H4'    | 24:R:81:THR:HG21  | 1.91                     | 0.52              |
| 21:O:71:ASP:HB3   | 21:O:86:ILE:HD12  | 1.91                     | 0.52              |
| 2:1:168:ARG:HH21  | 2:1:175:GLN:HG3   | 1.74                     | 0.52              |
| 11:A:30:U:H5'     | 11:A:31:A:OP2     | 2.10                     | 0.52              |
| 7:6:38:ARG:HE     | 11:A:1184:U:H5'   | 1.73                     | 0.52              |
| 11:A:128:A:OP1    | 16:F:142:ARG:NH2  | 2.41                     | 0.52              |
| 22:P:176:THR:HG22 | 22:P:214:TYR:HE1  | 1.74                     | 0.52              |
| 11:A:1564:G:H2'   | 11:A:1565:G:H5''  | 1.92                     | 0.52              |
| 17:I:62:VAL:HG22  | 17:I:77:HIS:CD2   | 2.45                     | 0.52              |
| 11:A:334:U:OP1    | 11:A:337:C:N4     | 2.36                     | 0.52              |
| 15:E:316:PHE:CG   | 15:E:316:PHE:O    | 2.63                     | 0.52              |
| 21:O:51:TYR:CE2   | 21:O:78:ARG:HA    | 2.45                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:A:494:C:C5     | 11:A:554:A:H2     | 2.28                     | 0.52              |
| 11:A:1255:A:C8    | 11:A:1255:A:H3'   | 2.44                     | 0.52              |
| 11:A:67:A:H2'     | 11:A:68:A:O4'     | 2.09                     | 0.52              |
| 15:E:99:LEU:HD12  | 15:E:198:PHE:HE1  | 1.73                     | 0.52              |
| 31:Y:78:GLN:NE2   | 31:Y:87:VAL:HG21  | 2.24                     | 0.52              |
| 28:V:165:ILE:HD11 | 28:V:198:ARG:HB2  | 1.91                     | 0.52              |
| 26:T:189:TYR:CD1  | 26:T:243:ILE:HD11 | 2.44                     | 0.52              |
| 25:S:89:HIS:HA    | 25:S:119:THR:HG21 | 1.91                     | 0.52              |
| 6:5:153:THR:O     | 24:R:92:VAL:HG22  | 2.10                     | 0.52              |
| 11:A:513:A:OP2    | 11:A:513:A:H4'    | 2.10                     | 0.52              |
| 7:6:42:THR:HG22   | 7:6:55:LEU:HD11   | 1.92                     | 0.52              |
| 11:A:521:U:O2'    | 11:A:522:C:O5'    | 2.26                     | 0.52              |
| 11:A:1255:A:H8    | 11:A:1255:A:H3'   | 1.73                     | 0.52              |
| 11:A:575:A:OP1    | 27:U:82:LYS:NZ    | 2.34                     | 0.52              |
| 12:B:42:Y5P:OP2   | 25:S:85:ARG:NH2   | 2.43                     | 0.52              |
| 11:A:185:U:OP1    | 11:A:431:A:O2'    | 2.28                     | 0.52              |
| 15:E:69:ASN:OD1   | 15:E:171:PRO:HB3  | 2.10                     | 0.52              |
| 2:1:114:LEU:HD13  | 2:1:141:PHE:CE1   | 2.45                     | 0.52              |
| 11:A:1290:A:O5'   | 23:Q:111:ARG:NH2  | 2.41                     | 0.52              |
| 11:A:164:A:H5'    | 27:U:31:PHE:CD2   | 2.45                     | 0.52              |
| 12:B:68:P5P:C6    | 12:B:69:Y5P:H4    | 2.39                     | 0.52              |
| 11:A:1499:C:H2'   | 11:A:1500:U:C6    | 2.45                     | 0.52              |
| 2:1:8:VAL:O       | 2:1:11:TRP:HB2    | 2.09                     | 0.52              |
| 11:A:1138:A:C2'   | 11:A:1139:A:H5''  | 2.40                     | 0.51              |
| 2:1:197:PRO:HG2   | 2:1:200:GLU:HG3   | 1.91                     | 0.51              |
| 6:5:185:PHE:CD2   | 24:R:132:PRO:HA   | 2.44                     | 0.51              |
| 11:A:351:G:H5'    | 11:A:352:C:C5     | 2.45                     | 0.51              |
| 17:I:74:HIS:CG    | 17:I:75:ARG:N     | 2.78                     | 0.51              |
| 15:E:292:HIS:O    | 15:E:295:CYS:HB3  | 2.10                     | 0.51              |
| 16:F:216:VAL:HG22 | 16:F:258:THR:HB   | 1.92                     | 0.51              |
| 30:X:38:ASP:O     | 30:X:98:GLN:HA    | 2.10                     | 0.51              |
| 30:X:41:GLN:HE21  | 30:X:94:VAL:HG11  | 1.75                     | 0.51              |
| 23:Q:64:ARG:HH11  | 23:Q:144:LYS:HB3  | 1.76                     | 0.51              |
| 11:A:861:U:C2     | 14:D:254:ASN:HB2  | 2.46                     | 0.51              |
| 15:E:317:PRO:HG2  | 15:E:320:PHE:CE1  | 2.42                     | 0.51              |
| 1:0:61:VAL:HG13   | 1:0:65:ASN:HD22   | 1.75                     | 0.51              |
| 18:J:53:TYR:HB2   | 23:Q:251:VAL:HG23 | 1.92                     | 0.51              |
| 19:K:33:PRO:HA    | 19:K:37:PRO:HD2   | 1.91                     | 0.51              |
| 11:A:178:U:C4     | 11:A:1029:C:H1'   | 2.46                     | 0.51              |
| 11:A:557:A:H2'    | 11:A:558:A:C2     | 2.45                     | 0.51              |
| 27:U:141:ILE:HG21 | 28:V:80:HIS:HE1   | 1.76                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:U:94:GLN:NE2   | 27:U:145:VAL:HG13 | 2.26                     | 0.51              |
| 16:F:97:HIS:CE1   | 16:F:101:ILE:HD11 | 2.45                     | 0.51              |
| 11:A:443:U:H4'    | 23:Q:133:ARG:NH1  | 2.26                     | 0.51              |
| 11:A:548:A:H5'    | 18:J:127:PRO:HA   | 1.92                     | 0.51              |
| 31:Y:58:CYS:HA    | 31:Y:76:VAL:HG12  | 1.93                     | 0.51              |
| 18:J:126:PHE:HB2  | 18:J:131:LEU:HD22 | 1.91                     | 0.51              |
| 12:B:33:Y5P:O5'   | 12:B:33:Y5P:H6    | 2.10                     | 0.51              |
| 11:A:391:U:H2'    | 11:A:392:A:H8     | 1.76                     | 0.51              |
| 21:O:55:PRO:HB3   | 21:O:77:ILE:HG23  | 1.92                     | 0.51              |
| 23:Q:250:ARG:O    | 23:Q:251:VAL:HB   | 2.11                     | 0.51              |
| 11:A:973:G:H3'    | 11:A:974:A:H5''   | 1.92                     | 0.51              |
| 17:I:74:HIS:CG    | 17:I:75:ARG:H     | 2.29                     | 0.50              |
| 16:F:280:TYR:OH   | 22:P:109:ARG:HD3  | 2.11                     | 0.50              |
| 11:A:48:U:O2'     | 11:A:49:A:H4'     | 2.11                     | 0.50              |
| 11:A:1568:C:H3'   | 11:A:1569:A:H3'   | 1.93                     | 0.50              |
| 11:A:397:A:H2'    | 11:A:398:A:H5'    | 1.93                     | 0.50              |
| 28:V:112:VAL:HG13 | 28:V:199:ILE:HG21 | 1.93                     | 0.50              |
| 15:E:197:HIS:NE2  | 15:E:318:THR:HG22 | 2.26                     | 0.50              |
| 25:S:176:ARG:HG2  | 25:S:177:ARG:H    | 1.76                     | 0.50              |
| 25:S:54:ARG:HH22  | 25:S:141:ILE:HG22 | 1.74                     | 0.50              |
| 11:A:861:U:O2     | 14:D:254:ASN:HB2  | 2.12                     | 0.50              |
| 14:D:227:ILE:HG12 | 14:D:235:MET:HB3  | 1.92                     | 0.50              |
| 4:3:126:GLN:NE2   | 4:3:146:VAL:HG13  | 2.25                     | 0.50              |
| 25:S:122:VAL:HG12 | 25:S:160:ARG:HD2  | 1.92                     | 0.50              |
| 10:9:83:GLY:H     | 11:A:1525:U:H5'   | 1.77                     | 0.50              |
| 11:A:195:U:O2'    | 11:A:1012:A:OP1   | 2.26                     | 0.50              |
| 27:U:54:THR:HG21  | 28:V:176:MET:N    | 2.16                     | 0.50              |
| 19:K:33:PRO:HB3   | 19:K:37:PRO:HG2   | 1.93                     | 0.50              |
| 11:A:1520:A:H2'   | 11:A:1521:A:O4'   | 2.11                     | 0.50              |
| 4:3:68:ILE:HD11   | 4:3:122:LEU:HD13  | 1.94                     | 0.50              |
| 11:A:1048:C:H2'   | 11:A:1325:U:C4'   | 2.41                     | 0.50              |
| 11:A:229:G:H2'    | 11:A:230:C:C6     | 2.46                     | 0.50              |
| 2:1:100:ARG:HH22  | 17:I:75:ARG:NE    | 2.08                     | 0.50              |
| 16:F:50:LYS:HD2   | 16:F:81:GLU:OE1   | 2.12                     | 0.50              |
| 14:D:114:PRO:HA   | 14:D:123:PHE:CE2  | 2.46                     | 0.50              |
| 6:5:138:ARG:HA    | 6:5:141:MET:HG2   | 1.94                     | 0.50              |
| 11:A:691:U:H1'    | 11:A:692:A:H5'    | 1.92                     | 0.50              |
| 21:O:95:ARG:O     | 21:O:96:MET:HB2   | 2.11                     | 0.50              |
| 19:K:54:ASN:HB3   | 19:K:58:LYS:HE3   | 1.93                     | 0.50              |
| 11:A:1291:G:O6    | 11:A:1297:C:O2'   | 2.26                     | 0.50              |
| 11:A:936:U:H4'    | 11:A:937:U:H3'    | 1.93                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 18:J:181:ILE:HD11 | 18:J:191:PHE:CE2  | 2.47                     | 0.50              |
| 7:6:26:THR:HB     | 11:A:1239:U:H3'   | 1.92                     | 0.50              |
| 19:K:115:LYS:O    | 19:K:119:GLU:HG3  | 2.12                     | 0.50              |
| 11:A:771:C:H2'    | 11:A:772:A:H5''   | 1.94                     | 0.50              |
| 11:A:656:U:H2'    | 11:A:657:U:C6     | 2.47                     | 0.50              |
| 2:1:163:ARG:HD3   | 2:1:205:GLY:H     | 1.77                     | 0.49              |
| 11:A:1512:A:C2'   | 11:A:1513:A:H5''  | 2.42                     | 0.49              |
| 11:A:390:A:O2'    | 11:A:391:U:O4'    | 2.29                     | 0.49              |
| 18:J:163:GLU:N    | 18:J:163:GLU:OE1  | 2.45                     | 0.49              |
| 11:A:187:C:H3'    | 28:V:181:ARG:NH2  | 2.27                     | 0.49              |
| 25:S:52:ASN:OD1   | 25:S:55:ASN:HB2   | 2.12                     | 0.49              |
| 11:A:894:A:H5'    | 11:A:963:A:H5''   | 1.94                     | 0.49              |
| 31:Y:126:THR:HB   | 31:Y:152:ARG:CZ   | 2.42                     | 0.49              |
| 19:K:49:PHE:HE1   | 19:K:80:ILE:HD13  | 1.77                     | 0.49              |
| 19:K:66:LEU:HD13  | 19:K:82:ILE:HG23  | 1.94                     | 0.49              |
| 2:1:177:HIS:NE2   | 2:1:183:ARG:HD2   | 2.26                     | 0.49              |
| 12:B:62:Y5P:H4A   | 12:B:63:Y5P:H4    | 1.94                     | 0.49              |
| 11:A:653:C:H3'    | 11:A:654:C:H6     | 1.77                     | 0.49              |
| 24:R:20:LEU:HB2   | 24:R:24:SER:OG    | 2.12                     | 0.49              |
| 21:O:85:LEU:HD23  | 21:O:137:VAL:HG11 | 1.94                     | 0.49              |
| 22:P:177:ALA:HA   | 22:P:222:TYR:CD1  | 2.46                     | 0.49              |
| 30:X:138:ASP:HB3  | 30:X:141:ARG:HB2  | 1.94                     | 0.49              |
| 11:A:693:U:H5''   | 11:A:693:U:H6     | 1.77                     | 0.49              |
| 26:T:71:PRO:O     | 26:T:213:GLN:HG2  | 2.12                     | 0.49              |
| 11:A:329:A:N3     | 11:A:330:A:H5''   | 2.26                     | 0.49              |
| 11:A:499:A:N6     | 11:A:544:C:OP2    | 2.45                     | 0.49              |
| 16:F:218:LEU:HD23 | 16:F:260:VAL:HB   | 1.94                     | 0.49              |
| 3:2:137:VAL:O     | 3:2:141:MET:HG3   | 2.12                     | 0.49              |
| 11:A:115:U:H3'    | 11:A:116:A:H5''   | 1.94                     | 0.49              |
| 11:A:159:A:H5'    | 11:A:160:A:OP2    | 2.12                     | 0.49              |
| 11:A:734:C:OP1    | 14:D:78:LYS:HD2   | 2.11                     | 0.49              |
| 11:A:415:U:H2'    | 11:A:416:G:C8     | 2.47                     | 0.49              |
| 23:Q:87:PHE:CD1   | 23:Q:169:PHE:HD1  | 2.30                     | 0.49              |
| 11:A:686:A:C3'    | 11:A:687:A:H4'    | 2.42                     | 0.49              |
| 15:E:53:LEU:HD21  | 15:E:61:VAL:HG21  | 1.95                     | 0.49              |
| 25:S:149:THR:HG21 | 25:S:151:TRP:CZ2  | 2.47                     | 0.49              |
| 3:2:104:TRP:HE3   | 3:2:144:LEU:HD23  | 1.77                     | 0.49              |
| 11:A:1555:C:H4'   | 26:T:86:ARG:HH12  | 1.76                     | 0.49              |
| 19:K:67:PRO:HD2   | 19:K:85:PRO:HA    | 1.95                     | 0.49              |
| 11:A:688:U:H1'    | 11:A:1003:G:H21   | 1.78                     | 0.49              |
| 1:0:90:TYR:HE2    | 1:0:92:LEU:HD21   | 1.77                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 7:6:14:LYS:H      | 7:6:35:SER:HB2    | 1.77                     | 0.49              |
| 11:A:15:A:H2'     | 11:A:16:A:H8      | 1.78                     | 0.49              |
| 11:A:674:A:H5'    | 11:A:675:C:OP2    | 2.13                     | 0.49              |
| 11:A:870:A:H5''   | 11:A:871:U:OP2    | 2.13                     | 0.49              |
| 11:A:1519:U:C5    | 20:N:177:ARG:HG3  | 2.47                     | 0.49              |
| 3:2:242:HIS:NE2   | 31:Y:47:GLU:OE1   | 2.41                     | 0.49              |
| 11:A:841:C:OP1    | 14:D:264:ASN:ND2  | 2.43                     | 0.49              |
| 15:E:206:VAL:HG13 | 15:E:297:VAL:HG13 | 1.95                     | 0.49              |
| 11:A:351:G:H5'    | 11:A:352:C:H5     | 1.78                     | 0.49              |
| 25:S:72:TRP:CD1   | 25:S:73:PRO:HA    | 2.48                     | 0.49              |
| 7:6:45:HIS:CG     | 7:6:46:TYR:H      | 2.31                     | 0.49              |
| 22:P:186:ILE:HG12 | 22:P:193:PHE:CD1  | 2.47                     | 0.49              |
| 11:A:1028:G:H5'   | 11:A:1029:C:H5    | 1.78                     | 0.49              |
| 26:T:75:PHE:CD2   | 26:T:110:GLU:HG3  | 2.48                     | 0.49              |
| 31:Y:92:ASN:HD22  | 31:Y:115:LEU:HD21 | 1.77                     | 0.49              |
| 25:S:107:THR:HG21 | 25:S:119:THR:CG2  | 2.42                     | 0.49              |
| 31:Y:59:GLY:N     | 31:Y:76:VAL:O     | 2.46                     | 0.49              |
| 11:A:1543:A:H5'   | 11:A:1544:U:OP2   | 2.12                     | 0.49              |
| 11:A:63:A:N3      | 11:A:63:A:H2'     | 2.28                     | 0.49              |
| 2:1:58:GLN:HG3    | 22:P:89:PHE:CZ    | 2.48                     | 0.48              |
| 11:A:1517:U:OP2   | 11:A:1518:U:O2'   | 2.30                     | 0.48              |
| 3:2:115:LEU:O     | 3:2:118:GLU:HB3   | 2.12                     | 0.48              |
| 11:A:741:U:H3'    | 11:A:742:A:H5''   | 1.93                     | 0.48              |
| 11:A:70:A:H3'     | 11:A:71:U:C6      | 2.48                     | 0.48              |
| 11:A:844:C:C2'    | 11:A:845:U:H5''   | 2.43                     | 0.48              |
| 15:E:208:ALA:HB3  | 15:E:290:PRO:O    | 2.13                     | 0.48              |
| 6:5:136:GLU:HG2   | 6:5:177:ARG:HH22  | 1.77                     | 0.48              |
| 7:6:36:ARG:HD3    | 11:A:1183:A:OP1   | 2.14                     | 0.48              |
| 21:O:69:VAL:HG23  | 21:O:89:HIS:CE1   | 2.48                     | 0.48              |
| 15:E:175:LYS:HD2  | 15:E:296:LEU:HB3  | 1.94                     | 0.48              |
| 20:N:114:LYS:HA   | 20:N:118:ARG:NH1  | 2.27                     | 0.48              |
| 25:S:145:VAL:HG22 | 25:S:174:GLU:HB2  | 1.94                     | 0.48              |
| 11:A:924:U:O2'    | 11:A:925:A:C8     | 2.65                     | 0.48              |
| 11:A:115:U:H3'    | 11:A:116:A:C5'    | 2.44                     | 0.48              |
| 11:A:340:G:H2'    | 11:A:341:C:C6     | 2.49                     | 0.48              |
| 11:A:70:A:H5'     | 11:A:71:U:OP2     | 2.13                     | 0.48              |
| 24:R:110:ILE:HG23 | 24:R:111:PRO:HD2  | 1.95                     | 0.48              |
| 11:A:1349:U:H2'   | 11:A:1351:C:H5''  | 1.95                     | 0.48              |
| 26:T:75:PHE:HD2   | 26:T:110:GLU:HG3  | 1.78                     | 0.48              |
| 11:A:1418:A:H4'   | 14:D:278:ARG:HH12 | 1.78                     | 0.48              |
| 14:D:198:GLU:OE2  | 14:D:203:ARG:N    | 2.46                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:A:520:A:OP1    | 19:K:106:LYS:HE3  | 2.14                     | 0.48              |
| 11:A:925:A:H2'    | 11:A:926:G:O4'    | 2.13                     | 0.48              |
| 11:A:1329:G:HO2'  | 11:A:1375:U:HO2'  | 1.60                     | 0.48              |
| 31:Y:159:PHE:CG   | 31:Y:160:PRO:HD2  | 2.47                     | 0.48              |
| 9:8:113:ARG:NH2   | 11:A:84:G:OP1     | 2.46                     | 0.48              |
| 12:B:25:P5P:H5'1  | 12:B:25:P5P:H8    | 1.96                     | 0.48              |
| 26:T:87:THR:HG21  | 26:T:91:LYS:HD3   | 1.95                     | 0.48              |
| 26:T:139:GLN:HE21 | 26:T:150:ILE:HD12 | 1.78                     | 0.48              |
| 11:A:1536:A:H3'   | 11:A:1537:C:H6    | 1.78                     | 0.48              |
| 28:V:140:VAL:HG21 | 28:V:158:VAL:HG21 | 1.95                     | 0.48              |
| 11:A:479:G:N2     | 11:A:480:A:H1'    | 2.29                     | 0.48              |
| 15:E:102:LEU:HD23 | 15:E:296:LEU:HD13 | 1.96                     | 0.48              |
| 15:E:275:ARG:HD2  | 15:E:333:TYR:CE1  | 2.49                     | 0.48              |
| 11:A:1423:A:H5'   | 13:C:75:C:OP1     | 2.14                     | 0.48              |
| 22:P:127:VAL:HG11 | 22:P:138:VAL:HG22 | 1.96                     | 0.48              |
| 31:Y:138:THR:HG22 | 31:Y:139:GLU:H    | 1.79                     | 0.48              |
| 2:1:25:PRO:HB2    | 2:1:27:HIS:CE1    | 2.49                     | 0.48              |
| 17:I:109:GLY:HA2  | 17:I:140:PHE:HE2  | 1.78                     | 0.48              |
| 11:A:1236:A:H5'   | 11:A:1237:A:OP1   | 2.14                     | 0.48              |
| 17:I:124:LEU:HD13 | 17:I:131:TYR:CZ   | 2.48                     | 0.48              |
| 24:R:23:GLU:HG3   | 26:T:264:TRP:CZ3  | 2.49                     | 0.48              |
| 31:Y:94:HIS:ND1   | 31:Y:113:ALA:HB2  | 2.29                     | 0.48              |
| 24:R:38:ARG:HB2   | 24:R:85:LEU:HD11  | 1.96                     | 0.48              |
| 22:P:233:ARG:HE   | 22:P:244:LEU:HD11 | 1.79                     | 0.48              |
| 1:0:50:ARG:NH1    | 11:A:1198:A:OP1   | 2.47                     | 0.48              |
| 30:X:14:ASN:ND2   | 31:Y:210:HIS:HA   | 2.29                     | 0.48              |
| 19:K:94:ALA:HB1   | 19:K:116:HIS:CD2  | 2.46                     | 0.47              |
| 14:D:291:PRO:HA   | 14:D:292:PRO:HD3  | 1.74                     | 0.47              |
| 6:5:81:PRO:HA     | 11:A:1436:U:C2    | 2.49                     | 0.47              |
| 15:E:58:VAL:HG21  | 24:R:139:ARG:HH21 | 1.78                     | 0.47              |
| 18:J:136:GLU:HG2  | 18:J:144:LEU:HD11 | 1.96                     | 0.47              |
| 25:S:91:GLU:HG3   | 25:S:106:SER:HB3  | 1.96                     | 0.47              |
| 18:J:95:MET:HG3   | 18:J:181:ILE:HG12 | 1.96                     | 0.47              |
| 11:A:358:G:H5'    | 22:P:42:GLY:HA2   | 1.96                     | 0.47              |
| 9:8:124:ARG:NH2   | 11:A:1202:A:OP1   | 2.47                     | 0.47              |
| 28:V:153:LEU:HA   | 28:V:153:LEU:HD12 | 1.70                     | 0.47              |
| 18:J:187:SER:O    | 18:J:191:PHE:HD1  | 1.97                     | 0.47              |
| 11:A:329:A:H8     | 11:A:828:U:O2'    | 1.97                     | 0.47              |
| 6:5:146:GLY:HA3   | 6:5:150:ARG:NH2   | 2.28                     | 0.47              |
| 27:U:98:ASN:O     | 27:U:102:LEU:HB2  | 2.14                     | 0.47              |
| 11:A:1024:A:C6    | 11:A:1319:C:H1'   | 2.49                     | 0.47              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 31:Y:126:THR:HB  | 31:Y:152:ARG:NH1  | 2.30                     | 0.47              |
| 4:3:84:ASP:O     | 4:3:88:MET:HG2    | 2.14                     | 0.47              |
| 11:A:1445:A:H5'' | 11:A:1446:A:OP1   | 2.15                     | 0.47              |
| 27:U:24:VAL:HG11 | 27:U:39:TYR:CE1   | 2.48                     | 0.47              |
| 11:A:1397:G:O2'  | 11:A:1400:C:OP2   | 2.30                     | 0.47              |
| 11:A:845:U:H5'   | 11:A:845:U:C6     | 2.38                     | 0.47              |
| 5:4:52:LEU:CG    | 5:4:68:ARG:HB3    | 2.43                     | 0.47              |
| 11:A:618:A:HO2'  | 11:A:619:U:H6     | 1.61                     | 0.47              |
| 3:2:204:MET:HB3  | 3:2:205:PRO:HD2   | 1.97                     | 0.47              |
| 14:D:142:LEU:HB2 | 14:D:151:TRP:CZ3  | 2.50                     | 0.47              |
| 11:A:1290:A:N6   | 11:A:1302:G:O2'   | 2.47                     | 0.47              |
| 3:2:239:LYS:HZ1  | 31:Y:45:PRO:HG3   | 1.79                     | 0.47              |
| 11:A:397:A:C3'   | 11:A:398:A:H5'    | 2.45                     | 0.47              |
| 11:A:1519:U:H3'  | 11:A:1520:A:H5'   | 1.96                     | 0.47              |
| 6:5:83:ASN:ND2   | 11:A:1013:C:H41   | 2.12                     | 0.47              |
| 30:X:28:LEU:HD13 | 30:X:42:PHE:CE1   | 2.49                     | 0.47              |
| 11:A:697:G:H2'   | 11:A:698:A:C8     | 2.49                     | 0.47              |
| 24:R:15:PHE:HD1  | 24:R:25:ARG:HH22  | 1.62                     | 0.47              |
| 14:D:148:ARG:HD3 | 14:D:150:ARG:HD2  | 1.97                     | 0.47              |
| 11:A:2:C:OP1     | 29:W:48:LYS:N     | 2.47                     | 0.47              |
| 31:Y:74:GLY:HA3  | 31:Y:91:LEU:HD11  | 1.96                     | 0.47              |
| 19:K:23:ILE:HG12 | 19:K:67:PRO:HB3   | 1.96                     | 0.47              |
| 3:2:190:TRP:HB3  | 31:Y:216:TYR:CZ   | 2.49                     | 0.47              |
| 12:B:13:Y5P:N3   | 12:B:23:P5P:N1    | 2.63                     | 0.47              |
| 11:A:16:A:H1'    | 11:A:101:U:H5     | 1.80                     | 0.47              |
| 11:A:580:C:H5''  | 27:U:69:ILE:HD13  | 1.97                     | 0.47              |
| 22:P:114:GLN:HB3 | 22:P:115:PRO:HD2  | 1.96                     | 0.47              |
| 21:O:82:LYS:HA   | 21:O:82:LYS:HD2   | 1.75                     | 0.47              |
| 31:Y:44:VAL:HG11 | 31:Y:83:ARG:NE    | 2.30                     | 0.47              |
| 11:A:522:C:H5    | 11:A:530:A:H5''   | 1.80                     | 0.47              |
| 11:A:613:G:H1'   | 11:A:617:C:O2     | 2.15                     | 0.47              |
| 11:A:1541:U:OP2  | 15:E:141:ARG:HD2  | 2.15                     | 0.47              |
| 28:V:136:LYS:HB3 | 28:V:152:LEU:HD21 | 1.97                     | 0.47              |
| 11:A:62:C:OP1    | 17:I:76:ARG:NH1   | 2.48                     | 0.47              |
| 20:N:116:LEU:HA  | 20:N:116:LEU:HD23 | 1.76                     | 0.47              |
| 3:2:228:LEU:HA   | 3:2:228:LEU:HD23  | 1.70                     | 0.47              |
| 10:9:83:GLY:N    | 11:A:1525:U:H5'   | 2.30                     | 0.47              |
| 30:X:80:ARG:HD2  | 30:X:84:ASN:OD1   | 2.15                     | 0.47              |
| 18:J:117:ARG:HD3 | 18:J:117:ARG:HA   | 1.71                     | 0.47              |
| 11:A:1371:U:C2'  | 11:A:1372:U:H5'   | 2.45                     | 0.46              |
| 22:P:232:ALA:O   | 22:P:235:GLU:HB3  | 2.14                     | 0.46              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 11:A:1485:C:OP1  | 26:T:141:SER:HB3  | 2.15                     | 0.46              |
| 4:3:72:ILE:HD11  | 4:3:118:ARG:HB2   | 1.96                     | 0.46              |
| 11:A:806:G:H2'   | 11:A:807:G:H5''   | 1.97                     | 0.46              |
| 11:A:528:A:O2'   | 11:A:545:A:N1     | 2.48                     | 0.46              |
| 11:A:363:A:O2'   | 11:A:384:U:H5''   | 2.14                     | 0.46              |
| 11:A:386:A:H3'   | 11:A:387:A:H5''   | 1.97                     | 0.46              |
| 11:A:481:G:H2'   | 11:A:482:U:O4'    | 2.14                     | 0.46              |
| 11:A:883:G:H3'   | 11:A:884:A:H8     | 1.80                     | 0.46              |
| 21:O:77:ILE:HG22 | 21:O:78:ARG:HG3   | 1.97                     | 0.46              |
| 11:A:478:A:N1    | 29:W:208:HIS:HA   | 2.31                     | 0.46              |
| 11:A:374:U:H2'   | 11:A:374:U:O2     | 2.14                     | 0.46              |
| 11:A:1510:U:C2'  | 11:A:1511:U:H5''  | 2.45                     | 0.46              |
| 17:I:91:LYS:HE2  | 17:I:116:LYS:HB2  | 1.98                     | 0.46              |
| 20:N:25:MET:HB3  | 20:N:25:MET:HE2   | 1.89                     | 0.46              |
| 7:6:23:GLN:HE21  | 7:6:55:LEU:HB3    | 1.79                     | 0.46              |
| 25:S:81:LEU:HB2  | 25:S:144:MET:SD   | 2.55                     | 0.46              |
| 28:V:90:LEU:HD22 | 28:V:95:ARG:HD2   | 1.98                     | 0.46              |
| 11:A:895:A:H2'   | 11:A:896:C:C6     | 2.49                     | 0.46              |
| 11:A:718:C:OP2   | 14:D:149:LYS:NZ   | 2.39                     | 0.46              |
| 24:R:25:ARG:NH2  | 24:R:51:GLU:OE2   | 2.49                     | 0.46              |
| 21:O:41:VAL:HG12 | 21:O:119:ILE:HG23 | 1.97                     | 0.46              |
| 11:A:196:U:H2'   | 11:A:197:U:C6     | 2.50                     | 0.46              |
| 18:J:143:LEU:HB3 | 18:J:147:PHE:HE2  | 1.81                     | 0.46              |
| 28:V:180:LYS:O   | 28:V:181:ARG:HG2  | 2.15                     | 0.46              |
| 11:A:1502:A:H4'  | 11:A:1503:G:OP2   | 2.15                     | 0.46              |
| 24:R:46:TRP:HD1  | 24:R:122:ALA:HB2  | 1.80                     | 0.46              |
| 11:A:177:C:O2'   | 27:U:55:ARG:NH1   | 2.49                     | 0.46              |
| 2:1:83:GLU:OE2   | 2:1:128:THR:HG21  | 2.16                     | 0.46              |
| 11:A:1139:A:H2'  | 11:A:1140:U:C6    | 2.50                     | 0.46              |
| 11:A:1140:U:H2'  | 11:A:1141:U:C6    | 2.51                     | 0.46              |
| 23:Q:96:TYR:HB3  | 23:Q:151:VAL:HG11 | 1.97                     | 0.46              |
| 19:K:91:LEU:HD13 | 19:K:148:ALA:HA   | 1.98                     | 0.46              |
| 14:D:141:ALA:HB2 | 14:D:154:ALA:HB2  | 1.97                     | 0.46              |
| 20:N:59:ILE:HB   | 20:N:127:LEU:HD23 | 1.98                     | 0.46              |
| 26:T:76:LEU:HD13 | 26:T:283:TRP:CE3  | 2.51                     | 0.46              |
| 11:A:935:C:H3'   | 11:A:936:U:H2'    | 1.98                     | 0.46              |
| 21:O:90:ARG:H    | 21:O:103:ASN:ND2  | 2.14                     | 0.46              |
| 15:E:49:TRP:CD1  | 15:E:155:PHE:HB3  | 2.50                     | 0.46              |
| 22:P:207:PRO:O   | 22:P:211:VAL:HG23 | 2.15                     | 0.46              |
| 11:A:275:G:N7    | 14:D:260:LYS:HB2  | 2.30                     | 0.46              |
| 6:5:122:LEU:HD21 | 24:R:108:LEU:HD13 | 1.98                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:D:217:LEU:HD11 | 14:D:225:ALA:HB1  | 1.98                     | 0.46              |
| 27:U:116:LEU:HD21 | 28:V:148:LEU:HD11 | 1.97                     | 0.46              |
| 11:A:833:A:H5''   | 11:A:1429:G:H4'   | 1.98                     | 0.46              |
| 11:A:1139:A:H8    | 11:A:1139:A:H5'   | 1.80                     | 0.46              |
| 11:A:937:U:H4'    | 11:A:938:G:OP2    | 2.16                     | 0.46              |
| 1:0:53:ILE:HD11   | 1:0:99:TYR:OH     | 2.16                     | 0.46              |
| 11:A:940:U:H2'    | 11:A:941:C:C6     | 2.51                     | 0.46              |
| 16:F:181:LYS:HD3  | 16:F:181:LYS:HA   | 1.70                     | 0.46              |
| 2:1:40:PRO:HB3    | 2:1:43:TYR:CZ     | 2.51                     | 0.46              |
| 6:5:185:PHE:CE2   | 24:R:132:PRO:HA   | 2.51                     | 0.45              |
| 11:A:624:G:O4'    | 16:F:154:GLY:HA2  | 2.15                     | 0.45              |
| 20:N:20:LEU:HB2   | 20:N:141:LEU:HD13 | 1.98                     | 0.45              |
| 17:I:74:HIS:HB3   | 17:I:77:HIS:CE1   | 2.51                     | 0.45              |
| 2:1:58:GLN:HG3    | 22:P:89:PHE:CE1   | 2.52                     | 0.45              |
| 11:A:1527:A:H5'   | 11:A:1528:C:OP2   | 2.17                     | 0.45              |
| 25:S:59:LEU:HB3   | 25:S:61:VAL:HG23  | 1.97                     | 0.45              |
| 12:B:38:P5P:H2'   | 12:B:39:P5P:H8    | 1.98                     | 0.45              |
| 11:A:962:A:O2'    | 11:A:965:G:N3     | 2.39                     | 0.45              |
| 18:J:143:LEU:HB3  | 18:J:147:PHE:CE2  | 2.52                     | 0.45              |
| 11:A:1519:U:H5    | 20:N:177:ARG:HG3  | 1.79                     | 0.45              |
| 29:W:194:ALA:O    | 29:W:198:ILE:HG12 | 2.16                     | 0.45              |
| 11:A:786:A:N6     | 34:A:5158:HOH:O   | 2.46                     | 0.45              |
| 14:D:198:GLU:HG3  | 14:D:204:GLY:O    | 2.16                     | 0.45              |
| 14:D:197:VAL:HG11 | 14:D:227:ILE:HD13 | 1.98                     | 0.45              |
| 25:S:72:TRP:CG    | 25:S:73:PRO:HA    | 2.51                     | 0.45              |
| 15:E:111:THR:HG23 | 15:E:113:ASP:H    | 1.82                     | 0.45              |
| 30:X:58:GLU:HG2   | 30:X:63:VAL:O     | 2.16                     | 0.45              |
| 2:1:227:PHE:HB2   | 3:2:158:LEU:O     | 2.17                     | 0.45              |
| 1:0:102:GLU:HB2   | 1:0:130:PHE:CE2   | 2.51                     | 0.45              |
| 4:3:38:ARG:HB2    | 11:A:409:U:OP1    | 2.16                     | 0.45              |
| 18:J:181:ILE:HB   | 18:J:186:LEU:HD12 | 1.98                     | 0.45              |
| 19:K:68:THR:OG1   | 19:K:80:ILE:HD11  | 2.16                     | 0.45              |
| 11:A:1312:U:C5'   | 11:A:1391:C:H5''  | 2.42                     | 0.45              |
| 15:E:197:HIS:CD2  | 15:E:318:THR:HG22 | 2.52                     | 0.45              |
| 11:A:549:A:P      | 18:J:128:ASN:HB2  | 2.56                     | 0.45              |
| 11:A:617:C:O3'    | 11:A:618:A:H8     | 2.00                     | 0.45              |
| 11:A:1519:U:O2'   | 20:N:177:ARG:NH2  | 2.49                     | 0.45              |
| 25:S:71:VAL:HG12  | 25:S:72:TRP:H     | 1.82                     | 0.45              |
| 6:5:152:PRO:HG3   | 6:5:173:ARG:NH1   | 2.31                     | 0.45              |
| 31:Y:98:VAL:HB    | 31:Y:107:THR:HB   | 1.98                     | 0.45              |
| 14:D:95:GLY:HA2   | 14:D:270:ARG:HB2  | 1.98                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:D:164:VAL:HG13 | 14:D:180:GLY:O    | 2.16                     | 0.45              |
| 18:J:156:SER:HB3  | 18:J:159:PRO:CB   | 2.37                     | 0.45              |
| 16:F:283:LEU:HB2  | 22:P:125:ARG:NH1  | 2.31                     | 0.45              |
| 11:A:58:C:C2'     | 11:A:59:A:H5''    | 2.46                     | 0.45              |
| 29:W:155:ARG:HD2  | 29:W:165:MET:SD   | 2.57                     | 0.45              |
| 28:V:139:LEU:HD12 | 28:V:147:LEU:O    | 2.16                     | 0.45              |
| 4:3:88:MET:CE     | 11:A:416:G:H21    | 2.29                     | 0.45              |
| 22:P:40:PRO:HA    | 22:P:45:ARG:HB3   | 1.98                     | 0.45              |
| 27:U:89:ASN:ND2   | 27:U:124:ARG:HB2  | 2.32                     | 0.45              |
| 11:A:789:A:O3'    | 15:E:238:ARG:HB2  | 2.16                     | 0.45              |
| 21:O:31:ALA:HA    | 21:O:66:VAL:HG13  | 1.99                     | 0.45              |
| 11:A:581:A:H5'    | 11:A:582:A:OP1    | 2.16                     | 0.45              |
| 15:E:97:VAL:HG21  | 15:E:187:ILE:HD11 | 1.98                     | 0.45              |
| 31:Y:129:LYS:HD3  | 31:Y:149:ARG:NH2  | 2.29                     | 0.45              |
| 11:A:875:U:HO2'   | 11:A:876:G:P      | 2.37                     | 0.45              |
| 11:A:1373:U:C2    | 11:A:1375:U:H5''  | 2.51                     | 0.45              |
| 11:A:41:A:H2'     | 11:A:42:C:H4'     | 1.97                     | 0.45              |
| 11:A:993:C:C5'    | 24:R:13:ARG:HH22  | 2.25                     | 0.45              |
| 5:4:58:VAL:HB     | 5:4:77:THR:HG23   | 1.99                     | 0.45              |
| 2:1:128:THR:HG22  | 2:1:129:MET:H     | 1.81                     | 0.45              |
| 15:E:90:TRP:HD1   | 15:E:316:PHE:CD2  | 2.35                     | 0.45              |
| 28:V:112:VAL:CG1  | 28:V:199:ILE:HG12 | 2.46                     | 0.45              |
| 16:F:106:PHE:CE1  | 16:F:107:LYS:HG3  | 2.52                     | 0.45              |
| 6:5:106:ASN:O     | 6:5:119:LYS:HG3   | 2.17                     | 0.45              |
| 27:U:54:THR:HG22  | 28:V:175:ASN:HA   | 1.98                     | 0.45              |
| 6:5:138:ARG:HB3   | 11:A:653:C:O2     | 2.16                     | 0.45              |
| 18:J:135:LEU:HD22 | 18:J:140:TYR:HB2  | 1.99                     | 0.45              |
| 23:Q:250:ARG:HD2  | 23:Q:250:ARG:HA   | 1.77                     | 0.45              |
| 11:A:102:G:O2'    | 11:A:103:A:H5'    | 2.17                     | 0.45              |
| 11:A:1518:U:H6    | 11:A:1518:U:O5'   | 2.00                     | 0.45              |
| 1:0:67:LEU:N      | 1:0:89:LEU:O      | 2.37                     | 0.45              |
| 15:E:348:THR:HA   | 26:T:129:LYS:HE3  | 1.98                     | 0.45              |
| 31:Y:133:VAL:CG1  | 31:Y:145:ARG:HB3  | 2.47                     | 0.45              |
| 31:Y:127:ASP:OD1  | 31:Y:152:ARG:NH1  | 2.50                     | 0.45              |
| 30:X:14:ASN:HD21  | 31:Y:211:LYS:H    | 1.65                     | 0.45              |
| 22:P:191:VAL:HB   | 22:P:192:PRO:HD3  | 1.98                     | 0.45              |
| 11:A:235:U:H5'    | 11:A:236:A:OP2    | 2.17                     | 0.45              |
| 11:A:1055:A:H5''  | 11:A:1056:C:OP2   | 2.16                     | 0.45              |
| 11:A:1159:G:H4'   | 11:A:1227:A:H5'   | 1.99                     | 0.45              |
| 11:A:732:A:OP2    | 14:D:105:ARG:NH2  | 2.50                     | 0.45              |
| 11:A:524:A:O2'    | 19:K:135:VAL:HG21 | 2.16                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:A:203:G:N3     | 11:A:203:G:H2'    | 2.31                     | 0.45              |
| 2:1:189:ASP:O     | 2:1:192:LYS:HB2   | 2.17                     | 0.45              |
| 11:A:502:G:H2'    | 11:A:503:U:C6     | 2.52                     | 0.44              |
| 11:A:163:A:O2'    | 11:A:1014:C:H5    | 1.99                     | 0.44              |
| 31:Y:25:ARG:HA    | 31:Y:26:PRO:HD2   | 1.82                     | 0.44              |
| 22:P:54:LYS:HB3   | 22:P:55:GLY:H     | 1.50                     | 0.44              |
| 11:A:530:A:N3     | 11:A:530:A:H2'    | 2.32                     | 0.44              |
| 11:A:556:C:O2'    | 11:A:557:A:OP2    | 2.32                     | 0.44              |
| 11:A:1164:A:N6    | 11:A:1171:A:OP2   | 2.43                     | 0.44              |
| 16:F:96:LEU:HD23  | 16:F:96:LEU:HA    | 1.82                     | 0.44              |
| 27:U:64:LEU:HA    | 27:U:64:LEU:HD23  | 1.66                     | 0.44              |
| 11:A:476:A:C3'    | 11:A:477:G:H5''   | 2.47                     | 0.44              |
| 9:8:116:ARG:HH11  | 9:8:167:LYS:HG2   | 1.82                     | 0.44              |
| 11:A:196:U:H2'    | 11:A:197:U:H6     | 1.81                     | 0.44              |
| 16:F:114:THR:HB   | 16:F:155:PRO:HD2  | 1.99                     | 0.44              |
| 12:B:71:Y5P:H4A   | 12:B:72:Y5P:H4    | 1.98                     | 0.44              |
| 17:I:130:VAL:HB   | 17:I:136:ASN:HD21 | 1.82                     | 0.44              |
| 11:A:32:C:O2'     | 11:A:36:A:N6      | 2.50                     | 0.44              |
| 31:Y:62:VAL:HB    | 31:Y:120:VAL:HG13 | 1.98                     | 0.44              |
| 28:V:60:LEU:HA    | 28:V:60:LEU:HD23  | 1.70                     | 0.44              |
| 29:W:79:LYS:HA    | 29:W:79:LYS:HD2   | 1.86                     | 0.44              |
| 11:A:1028:G:H5'   | 11:A:1029:C:C5    | 2.52                     | 0.44              |
| 11:A:42:C:H5'     | 11:A:43:C:OP2     | 2.17                     | 0.44              |
| 26:T:99:MET:O     | 26:T:103:ARG:HG2  | 2.16                     | 0.44              |
| 11:A:420:U:H2'    | 11:A:421:U:C6     | 2.53                     | 0.44              |
| 16:F:168:LYS:HE3  | 16:F:279:ARG:HE   | 1.82                     | 0.44              |
| 16:F:191:ASP:O    | 16:F:192:SER:OG   | 2.28                     | 0.44              |
| 19:K:113:THR:HG22 | 19:K:114:LEU:H    | 1.82                     | 0.44              |
| 16:F:293:PHE:HA   | 16:F:294:PRO:HD3  | 1.85                     | 0.44              |
| 31:Y:196:GLU:H    | 31:Y:196:GLU:HG2  | 1.47                     | 0.44              |
| 8:7:95:HIS:HD2    | 11:A:124:A:H5''   | 1.82                     | 0.44              |
| 17:I:60:TRP:CG    | 17:I:76:ARG:HG3   | 2.52                     | 0.44              |
| 11:A:6:A:H5'      | 11:A:7:G:OP2      | 2.18                     | 0.44              |
| 11:A:393:C:H5'    | 11:A:394:C:OP2    | 2.17                     | 0.44              |
| 24:R:86:ILE:HB    | 24:R:87:PRO:HD3   | 2.00                     | 0.44              |
| 11:A:1138:A:H2'   | 11:A:1139:A:H5''  | 2.00                     | 0.44              |
| 27:U:14:VAL:HB    | 27:U:17:ARG:HH21  | 1.82                     | 0.44              |
| 11:A:473:A:N6     | 11:A:594:A:C6     | 2.85                     | 0.44              |
| 20:N:109:TYR:HA   | 20:N:122:MET:HE1  | 2.00                     | 0.44              |
| 15:E:193:LEU:HA   | 15:E:193:LEU:HD23 | 1.76                     | 0.44              |
| 11:A:816:A:H5''   | 11:A:816:A:H8     | 1.83                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:1:42:HIS:CE1    | 2:1:83:GLU:HB2    | 2.53                     | 0.44              |
| 22:P:220:ARG:NH2  | 22:P:233:ARG:HA   | 2.32                     | 0.44              |
| 11:A:913:C:H2'    | 11:A:914:C:H5'    | 1.99                     | 0.44              |
| 11:A:1374:G:H8    | 11:A:1374:G:OP1   | 2.01                     | 0.44              |
| 12:B:25:P5P:C6    | 12:B:26:Y5P:H4    | 2.47                     | 0.44              |
| 19:K:66:LEU:HA    | 19:K:85:PRO:HA    | 1.98                     | 0.44              |
| 11:A:549:A:OP1    | 18:J:128:ASN:HB2  | 2.17                     | 0.44              |
| 2:1:42:HIS:O      | 17:I:55:ILE:HA    | 2.18                     | 0.44              |
| 12:B:38:P5P:H2'   | 12:B:39:P5P:C8    | 2.48                     | 0.44              |
| 15:E:219:MET:SD   | 15:E:238:ARG:HD3  | 2.58                     | 0.44              |
| 17:I:130:VAL:HB   | 17:I:136:ASN:ND2  | 2.33                     | 0.44              |
| 29:W:151:LEU:HB2  | 29:W:167:LYS:HB2  | 2.00                     | 0.44              |
| 11:A:711:A:H4'    | 11:A:711:A:OP1    | 2.18                     | 0.44              |
| 11:A:1485:C:H1'   | 21:O:95:ARG:NH2   | 2.32                     | 0.44              |
| 11:A:1557:A:H4'   | 15:E:263:ASN:ND2  | 2.33                     | 0.44              |
| 15:E:112:LYS:HA   | 15:E:338:CYS:SG   | 2.58                     | 0.44              |
| 30:X:77:ASN:HA    | 30:X:77:ASN:HD22  | 1.59                     | 0.44              |
| 15:E:193:LEU:HD21 | 15:E:318:THR:HG21 | 2.00                     | 0.44              |
| 16:F:71:GLY:HA3   | 16:F:74:GLN:HG2   | 2.00                     | 0.44              |
| 23:Q:109:ILE:HD11 | 23:Q:176:LEU:HD21 | 2.00                     | 0.44              |
| 11:A:577:U:HO2'   | 11:A:578:A:P      | 2.38                     | 0.44              |
| 1:0:90:TYR:CE2    | 1:0:92:LEU:HD21   | 2.53                     | 0.44              |
| 4:3:128:LEU:HA    | 4:3:129:PRO:HD3   | 1.89                     | 0.44              |
| 26:T:197:TYR:CE2  | 26:T:222:VAL:HG13 | 2.53                     | 0.44              |
| 2:1:97:LEU:HA     | 2:1:97:LEU:HD23   | 1.79                     | 0.44              |
| 11:A:572:A:O2'    | 11:A:573:C:O5'    | 2.36                     | 0.43              |
| 15:E:187:ILE:HG22 | 15:E:188:LYS:N    | 2.29                     | 0.43              |
| 6:5:108:ASP:OD2   | 6:5:119:LYS:HE2   | 2.17                     | 0.43              |
| 8:7:77:THR:HG21   | 11:A:249:A:H5'    | 1.99                     | 0.43              |
| 28:V:88:ASN:ND2   | 28:V:208:LEU:O    | 2.51                     | 0.43              |
| 11:A:954:C:C2'    | 11:A:955:U:H5'    | 2.47                     | 0.43              |
| 24:R:113:ARG:HD3  | 24:R:121:MET:SD   | 2.58                     | 0.43              |
| 15:E:208:ALA:HB2  | 15:E:297:VAL:HG22 | 2.00                     | 0.43              |
| 12:B:25:P5P:O5'   | 25:S:86:THR:HG21  | 2.18                     | 0.43              |
| 21:O:128:ARG:NH1  | 26:T:126:ALA:HA   | 2.33                     | 0.43              |
| 11:A:1139:A:O2'   | 11:A:1140:U:OP1   | 2.35                     | 0.43              |
| 28:V:152:LEU:HD23 | 28:V:152:LEU:HA   | 1.84                     | 0.43              |
| 16:F:191:ASP:C    | 16:F:192:SER:HG   | 2.21                     | 0.43              |
| 28:V:105:PHE:CE2  | 28:V:120:ILE:HD13 | 2.52                     | 0.43              |
| 26:T:178:LYS:HB2  | 26:T:178:LYS:HE3  | 1.82                     | 0.43              |
| 18:J:95:MET:O     | 18:J:156:SER:HB2  | 2.18                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:S:126:GLU:CG   | 25:S:160:ARG:HB3  | 2.47                     | 0.43              |
| 31:Y:159:PHE:CD1  | 31:Y:160:PRO:HD2  | 2.53                     | 0.43              |
| 31:Y:98:VAL:HG21  | 31:Y:109:ILE:HD12 | 2.01                     | 0.43              |
| 20:N:80:HIS:CD2   | 20:N:82:GLY:H     | 2.37                     | 0.43              |
| 10:9:63:PHE:HD2   | 11:A:1347:G:HO2'  | 1.66                     | 0.43              |
| 10:9:94:LYS:HE2   | 11:A:1299:A:H5'   | 2.00                     | 0.43              |
| 14:D:185:LEU:HA   | 14:D:185:LEU:HD23 | 1.76                     | 0.43              |
| 11:A:476:A:H5''   | 11:A:476:A:H8     | 1.84                     | 0.43              |
| 3:2:126:LEU:HD23  | 30:X:111:PHE:CD1  | 2.53                     | 0.43              |
| 15:E:296:LEU:HD12 | 15:E:296:LEU:HA   | 1.74                     | 0.43              |
| 2:1:168:ARG:NH2   | 2:1:176:LEU:HA    | 2.33                     | 0.43              |
| 11:A:1197:A:H2'   | 11:A:1198:A:O4'   | 2.19                     | 0.43              |
| 11:A:275:G:C5     | 14:D:260:LYS:HB2  | 2.54                     | 0.43              |
| 26:T:197:TYR:CD2  | 26:T:222:VAL:HG13 | 2.53                     | 0.43              |
| 27:U:107:ILE:HD13 | 29:W:206:ILE:HG21 | 2.00                     | 0.43              |
| 26:T:100:LEU:HD23 | 26:T:100:LEU:HA   | 1.88                     | 0.43              |
| 22:P:178:PHE:CE2  | 22:P:206:PRO:HA   | 2.54                     | 0.43              |
| 11:A:570:A:OP1    | 20:N:107:ALA:HA   | 2.18                     | 0.43              |
| 11:A:68:A:N3      | 11:A:69:C:H5'     | 2.33                     | 0.43              |
| 18:J:162:LYS:HE3  | 18:J:195:SER:O    | 2.17                     | 0.43              |
| 11:A:959:A:H8     | 11:A:959:A:OP1    | 2.02                     | 0.43              |
| 11:A:1568:C:H5''  | 11:A:1569:A:H2'   | 2.00                     | 0.43              |
| 22:P:177:ALA:HB1  | 22:P:203:ARG:NH2  | 2.33                     | 0.43              |
| 27:U:87:ILE:O     | 27:U:91:ILE:HG13  | 2.18                     | 0.43              |
| 4:3:133:ASP:HB3   | 4:3:147:VAL:HG22  | 2.01                     | 0.43              |
| 25:S:68:TRP:CD1   | 25:S:75:ARG:HB2   | 2.54                     | 0.43              |
| 9:8:175:ASP:HB3   | 9:8:178:GLN:HB2   | 2.01                     | 0.43              |
| 18:J:108:ASP:O    | 18:J:112:LEU:HB2  | 2.18                     | 0.43              |
| 25:S:143:PHE:CD1  | 25:S:175:PRO:HD3  | 2.53                     | 0.43              |
| 11:A:809:A:N3     | 15:E:230:THR:HG21 | 2.33                     | 0.43              |
| 22:P:47:ARG:HD2   | 28:V:183:ASN:ND2  | 2.33                     | 0.43              |
| 9:8:115:LEU:HB2   | 22:P:83:PHE:CD1   | 2.53                     | 0.43              |
| 12:B:30:P5P:H3'   | 12:B:31:Y5P:H6    | 2.00                     | 0.43              |
| 2:1:161:LEU:HD12  | 2:1:161:LEU:HA    | 1.76                     | 0.43              |
| 14:D:170:ILE:HG21 | 14:D:239:GLU:OE2  | 2.18                     | 0.43              |
| 11:A:502:G:C6     | 11:A:523:A:C2     | 3.07                     | 0.43              |
| 11:A:428:G:C5'    | 22:P:57:ARG:HD3   | 2.47                     | 0.43              |
| 11:A:931:A:H1'    | 11:A:1426:U:O2'   | 2.19                     | 0.43              |
| 23:Q:211:ASN:HA   | 23:Q:212:PRO:HD3  | 1.80                     | 0.43              |
| 4:3:101:LYS:HE3   | 11:A:416:G:OP1    | 2.18                     | 0.43              |
| 11:A:421:U:H2'    | 11:A:422:U:C6     | 2.53                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 19:K:24:VAL:HB    | 19:K:53:PHE:CZ    | 2.54                     | 0.43              |
| 18:J:47:LEU:HD22  | 23:Q:226:ILE:HG13 | 2.01                     | 0.43              |
| 8:7:58:PRO:HG2    | 11:A:758:C:H5'    | 2.01                     | 0.43              |
| 11:A:1157:U:H1'   | 11:A:1249:C:H2'   | 2.00                     | 0.43              |
| 27:U:50:PHE:O     | 27:U:54:THR:HG23  | 2.19                     | 0.43              |
| 26:T:233:TRP:CE3  | 26:T:240:ILE:HD11 | 2.54                     | 0.43              |
| 1:0:92:LEU:HB3    | 25:S:66:ARG:HE    | 1.84                     | 0.43              |
| 11:A:772:A:H8     | 11:A:772:A:C5'    | 2.31                     | 0.43              |
| 26:T:99:MET:HB2   | 26:T:167:TYR:CE1  | 2.54                     | 0.43              |
| 16:F:168:LYS:HE3  | 16:F:279:ARG:HH21 | 1.83                     | 0.43              |
| 11:A:328:A:C2     | 14:D:275:LEU:HD13 | 2.52                     | 0.43              |
| 22:P:68:GLU:CG    | 22:P:73:PRO:HA    | 2.48                     | 0.43              |
| 30:X:112:PRO:O    | 30:X:113:GLU:HB2  | 2.18                     | 0.43              |
| 22:P:121:LEU:HD23 | 22:P:121:LEU:HA   | 1.83                     | 0.43              |
| 25:S:58:LEU:HD23  | 25:S:58:LEU:HA    | 1.77                     | 0.43              |
| 14:D:111:ARG:HD2  | 14:D:182:ALA:HB2  | 2.01                     | 0.43              |
| 11:A:1255:A:C8    | 11:A:1255:A:C3'   | 3.02                     | 0.43              |
| 11:A:501:A:H1'    | 11:A:524:A:C2     | 2.53                     | 0.43              |
| 23:Q:205:ARG:NH1  | 23:Q:249:GLU:HA   | 2.34                     | 0.43              |
| 22:P:118:LEU:HD23 | 22:P:187:LEU:HD23 | 2.01                     | 0.43              |
| 12:B:43:Y5P:H2'   | 12:B:44:Y5P:HB2   | 2.01                     | 0.43              |
| 7:6:38:ARG:NE     | 11:A:1184:U:H5'   | 2.33                     | 0.43              |
| 11:A:936:U:H4'    | 11:A:937:U:OP2    | 2.18                     | 0.43              |
| 11:A:101:U:O2'    | 11:A:102:G:O4'    | 2.30                     | 0.43              |
| 11:A:624:G:C5     | 27:U:11:ARG:HB2   | 2.53                     | 0.43              |
| 11:A:913:C:C2'    | 11:A:914:C:H5'    | 2.48                     | 0.43              |
| 23:Q:98:HIS:HD2   | 23:Q:100:GLY:H    | 1.67                     | 0.43              |
| 2:1:93:ASN:O      | 2:1:94:ASN:HB2    | 2.19                     | 0.43              |
| 8:7:84:ARG:NH1    | 11:A:126:G:OP1    | 2.52                     | 0.43              |
| 14:D:133:ASP:OD2  | 14:D:136:ARG:HG2  | 2.18                     | 0.43              |
| 31:Y:73:GLN:OE1   | 31:Y:123:VAL:HG21 | 2.19                     | 0.43              |
| 12:B:4:P5P:O5'    | 12:B:4:P5P:H8     | 2.19                     | 0.43              |
| 31:Y:19:TYR:OH    | 31:Y:26:PRO:HA    | 2.19                     | 0.42              |
| 27:U:87:ILE:HA    | 27:U:87:ILE:HD13  | 1.69                     | 0.42              |
| 3:2:119:GLN:NE2   | 11:A:700:A:OP1    | 2.50                     | 0.42              |
| 16:F:84:PRO:O     | 16:F:88:SER:HB3   | 2.18                     | 0.42              |
| 11:A:759:A:N1     | 11:A:763:C:H2'    | 2.33                     | 0.42              |
| 11:A:70:A:H3'     | 11:A:71:U:H6      | 1.84                     | 0.42              |
| 11:A:571:A:H5''   | 11:A:572:A:OP1    | 2.19                     | 0.42              |
| 16:F:221:LEU:HG   | 16:F:222:GLU:HG3  | 2.01                     | 0.42              |
| 10:9:69:LEU:HD11  | 10:9:85:TRP:O     | 2.18                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:Q:205:ARG:HH12 | 23:Q:249:GLU:HA   | 1.84                     | 0.42              |
| 25:S:163:HIS:O    | 25:S:167:GLU:HG2  | 2.19                     | 0.42              |
| 29:W:92:ILE:HD12  | 29:W:140:VAL:HG21 | 2.00                     | 0.42              |
| 19:K:139:SER:HA   | 19:K:142:ARG:HD2  | 2.02                     | 0.42              |
| 30:X:136:SER:HA   | 30:X:137:PRO:HD3  | 1.88                     | 0.42              |
| 27:U:29:ARG:HA    | 27:U:29:ARG:HD3   | 1.87                     | 0.42              |
| 11:A:704:A:OP2    | 30:X:50:ARG:NH2   | 2.26                     | 0.42              |
| 11:A:718:C:OP1    | 11:A:718:C:H6     | 2.02                     | 0.42              |
| 11:A:1544:U:H5''  | 11:A:1545:A:OP2   | 2.19                     | 0.42              |
| 11:A:162:C:H5     | 11:A:1011:A:H61   | 1.66                     | 0.42              |
| 31:Y:65:LEU:HD11  | 31:Y:121:LYS:HG3  | 2.01                     | 0.42              |
| 25:S:125:CYS:SG   | 25:S:157:SER:HB2  | 2.59                     | 0.42              |
| 11:A:1393:A:H8    | 11:A:1393:A:OP2   | 2.02                     | 0.42              |
| 2:1:16:LEU:HD11   | 2:1:29:LEU:HD22   | 2.01                     | 0.42              |
| 20:N:117:HIS:O    | 20:N:121:MET:HG2  | 2.19                     | 0.42              |
| 11:A:397:A:C2'    | 11:A:398:A:H5'    | 2.50                     | 0.42              |
| 25:S:144:MET:O    | 25:S:172:LEU:HA   | 2.19                     | 0.42              |
| 19:K:135:VAL:HG12 | 19:K:136:PRO:HD2  | 2.01                     | 0.42              |
| 15:E:149:GLY:O    | 15:E:173:LYS:HD2  | 2.19                     | 0.42              |
| 26:T:118:ARG:HA   | 26:T:133:PHE:O    | 2.19                     | 0.42              |
| 11:A:863:A:H2'    | 11:A:864:G:H8     | 1.84                     | 0.42              |
| 31:Y:66:GLU:HB3   | 31:Y:119:GLN:HB3  | 2.01                     | 0.42              |
| 11:A:799:G:H4'    | 21:O:36:THR:HG22  | 2.01                     | 0.42              |
| 11:A:150:A:H8     | 11:A:150:A:O5'    | 2.02                     | 0.42              |
| 23:Q:105:MET:O    | 23:Q:109:ILE:HB   | 2.19                     | 0.42              |
| 12:B:69:Y5P:H2'   | 12:B:70:P5P:O4'   | 2.20                     | 0.42              |
| 26:T:82:PRO:HA    | 26:T:83:PRO:HD3   | 1.77                     | 0.42              |
| 22:P:28:LYS:HA    | 22:P:29:PRO:HD2   | 1.91                     | 0.42              |
| 28:V:176:MET:HE2  | 28:V:176:MET:HB3  | 1.76                     | 0.42              |
| 26:T:76:LEU:HD13  | 26:T:283:TRP:CZ3  | 2.55                     | 0.42              |
| 28:V:165:ILE:CD1  | 28:V:198:ARG:HB2  | 2.49                     | 0.42              |
| 23:Q:72:ILE:HD11  | 23:Q:96:TYR:CZ    | 2.55                     | 0.42              |
| 11:A:255:U:H2'    | 11:A:256:A:H5'    | 2.01                     | 0.42              |
| 26:T:84:ARG:HG3   | 26:T:273:TYR:HE1  | 1.85                     | 0.42              |
| 1:0:35:THR:HG21   | 23:Q:138:GLN:OE1  | 2.20                     | 0.42              |
| 26:T:97:LYS:O     | 26:T:101:GLU:HG2  | 2.19                     | 0.42              |
| 26:T:190:LEU:HA   | 26:T:190:LEU:HD23 | 1.86                     | 0.42              |
| 4:3:73:LYS:HB3    | 4:3:73:LYS:HE2    | 1.43                     | 0.42              |
| 11:A:1547:A:N6    | 11:A:1548:U:O4    | 2.53                     | 0.42              |
| 11:A:890:G:O5'    | 11:A:890:G:H8     | 2.02                     | 0.42              |
| 23:Q:226:ILE:HD13 | 23:Q:226:ILE:HA   | 1.74                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:A:91:A:C8      | 11:A:92:U:C6      | 3.08                     | 0.42              |
| 7:6:50:VAL:HB     | 7:6:52:LYS:HG2    | 2.01                     | 0.42              |
| 28:V:91:ILE:HD12  | 28:V:204:ILE:HD13 | 2.02                     | 0.42              |
| 15:E:195:ALA:H    | 15:E:281:ASN:ND2  | 2.18                     | 0.42              |
| 9:8:95:THR:HB     | 9:8:105:LYS:HB2   | 2.00                     | 0.42              |
| 16:F:184:GLN:O    | 16:F:185:ASP:HB2  | 2.19                     | 0.42              |
| 31:Y:22:GLY:C     | 31:Y:24:SER:H     | 2.21                     | 0.42              |
| 28:V:85:GLY:O     | 28:V:89:GLU:HG2   | 2.20                     | 0.42              |
| 30:X:3:ARG:H      | 30:X:23:ASN:HB3   | 1.85                     | 0.42              |
| 22:P:160:SER:O    | 22:P:164:ILE:HG13 | 2.20                     | 0.42              |
| 12:B:3:Y5P:N3     | 12:B:67:P5P:N1    | 2.68                     | 0.42              |
| 14:D:175:VAL:HG11 | 14:D:183:HIS:CE1  | 2.54                     | 0.42              |
| 25:S:96:HIS:HD2   | 25:S:98:ASN:HB2   | 1.84                     | 0.42              |
| 11:A:993:C:H5''   | 24:R:13:ARG:NH2   | 2.27                     | 0.42              |
| 11:A:163:A:H3'    | 27:U:35:LYS:HZ2   | 1.84                     | 0.42              |
| 25:S:89:HIS:HA    | 25:S:119:THR:CG2  | 2.49                     | 0.42              |
| 30:X:141:ARG:HD2  | 30:X:141:ARG:HA   | 1.66                     | 0.42              |
| 11:A:673:U:H4'    | 11:A:674:A:H5''   | 2.01                     | 0.42              |
| 14:D:189:PRO:HD2  | 14:D:192:THR:HG21 | 2.01                     | 0.42              |
| 22:P:209:ALA:O    | 22:P:212:PRO:HD2  | 2.19                     | 0.42              |
| 3:2:75:ASN:OD1    | 3:2:81:VAL:HG11   | 2.20                     | 0.42              |
| 28:V:150:LYS:HA   | 28:V:151:PRO:HA   | 1.85                     | 0.42              |
| 11:A:929:U:C3'    | 11:A:930:A:H5'    | 2.50                     | 0.42              |
| 11:A:1339:A:N3    | 11:A:1339:A:H2'   | 2.34                     | 0.42              |
| 24:R:83:LYS:HD2   | 24:R:83:LYS:HA    | 1.81                     | 0.42              |
| 11:A:136:A:H5''   | 31:Y:85:TRP:CH2   | 2.55                     | 0.42              |
| 11:A:1209:A:OP1   | 25:S:176:ARG:NH2  | 2.49                     | 0.42              |
| 4:3:88:MET:H      | 4:3:88:MET:HG2    | 1.56                     | 0.42              |
| 14:D:74:VAL:HG13  | 14:D:151:TRP:NE1  | 2.35                     | 0.42              |
| 1:0:53:ILE:HD11   | 1:0:99:TYR:CZ     | 2.54                     | 0.42              |
| 11:A:954:C:H2'    | 11:A:955:U:H5'    | 2.02                     | 0.42              |
| 2:1:202:GLU:HG3   | 2:1:203:TRP:CD1   | 2.55                     | 0.42              |
| 11:A:1452:C:H2'   | 11:A:1453:C:O4'   | 2.20                     | 0.42              |
| 11:A:735:G:H2'    | 11:A:736:U:C6     | 2.55                     | 0.42              |
| 11:A:777:G:H5'    | 11:A:778:G:OP2    | 2.20                     | 0.42              |
| 11:A:671:C:O2'    | 11:A:757:C:H5''   | 2.20                     | 0.42              |
| 22:P:27:LEU:HA    | 22:P:27:LEU:HD23  | 1.88                     | 0.42              |
| 31:Y:127:ASP:HB3  | 31:Y:152:ARG:HH22 | 1.85                     | 0.42              |
| 15:E:99:LEU:HD12  | 15:E:198:PHE:CE1  | 2.53                     | 0.42              |
| 11:A:1048:C:O5'   | 11:A:1049:G:H5''  | 2.20                     | 0.42              |
| 1:0:77:PRO:HD2    | 25:S:70:THR:OG1   | 2.20                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:B:61:Y5P:H2'   | 12:B:62:Y5P:H6    | 2.01                     | 0.42              |
| 26:T:100:LEU:HD11 | 26:T:286:ILE:HG12 | 2.01                     | 0.42              |
| 11:A:1060:A:H3'   | 11:A:1061:U:H5''  | 2.01                     | 0.42              |
| 18:J:61:ASN:CG    | 18:J:62:PRO:HD2   | 2.40                     | 0.42              |
| 29:W:78:ILE:HG22  | 29:W:80:TYR:H     | 1.84                     | 0.42              |
| 26:T:112:TYR:O    | 26:T:115:SER:HB3  | 2.19                     | 0.42              |
| 10:9:71:LYS:HB3   | 10:9:76:CYS:HB2   | 2.02                     | 0.42              |
| 11:A:1194:G:H8    | 11:A:1194:G:O5'   | 2.03                     | 0.42              |
| 22:P:176:THR:HB   | 22:P:221:GLY:HA2  | 2.01                     | 0.41              |
| 18:J:69:PRO:O     | 18:J:71:PRO:HD3   | 2.20                     | 0.41              |
| 4:3:108:ALA:O     | 4:3:111:LYS:HB2   | 2.19                     | 0.41              |
| 14:D:125:GLU:HB3  | 14:D:143:VAL:HG13 | 2.02                     | 0.41              |
| 11:A:812:C:O2     | 11:A:812:C:H2'    | 2.20                     | 0.41              |
| 9:8:142:ARG:HA    | 9:8:145:ARG:NH1   | 2.35                     | 0.41              |
| 31:Y:105:ARG:HD3  | 31:Y:105:ARG:N    | 2.28                     | 0.41              |
| 10:9:69:LEU:HD13  | 10:9:87:ILE:HG12  | 2.02                     | 0.41              |
| 11:A:691:U:O2'    | 11:A:692:A:P      | 2.79                     | 0.41              |
| 26:T:115:SER:HB2  | 26:T:180:GLU:H    | 1.85                     | 0.41              |
| 17:I:115:LYS:HE3  | 17:I:117:SER:HB2  | 2.02                     | 0.41              |
| 11:A:356:U:H5''   | 11:A:357:U:OP1    | 2.20                     | 0.41              |
| 3:2:168:GLY:HA3   | 3:2:180:TRP:CZ2   | 2.55                     | 0.41              |
| 11:A:52:A:H4'     | 11:A:244:A:H2     | 1.85                     | 0.41              |
| 27:U:90:LEU:HA    | 27:U:90:LEU:HD12  | 1.72                     | 0.41              |
| 2:1:156:LYS:HA    | 2:1:156:LYS:HD2   | 1.85                     | 0.41              |
| 11:A:530:A:H61    | 19:K:150:SER:HB3  | 1.85                     | 0.41              |
| 24:R:132:PRO:HA   | 24:R:133:PRO:HD3  | 1.96                     | 0.41              |
| 25:S:149:THR:HG21 | 25:S:151:TRP:CH2  | 2.56                     | 0.41              |
| 20:N:20:LEU:HD12  | 20:N:58:VAL:O     | 2.19                     | 0.41              |
| 21:O:33:GLN:H     | 21:O:36:THR:HG21  | 1.86                     | 0.41              |
| 11:A:119:A:H3'    | 11:A:120:C:H6     | 1.86                     | 0.41              |
| 9:8:140:ARG:HD2   | 11:A:1204:U:OP1   | 2.21                     | 0.41              |
| 21:O:107:LEU:HA   | 21:O:107:LEU:HD23 | 1.75                     | 0.41              |
| 22:P:51:ARG:HD3   | 22:P:51:ARG:HA    | 1.86                     | 0.41              |
| 16:F:274:LEU:HA   | 16:F:274:LEU:HD23 | 1.85                     | 0.41              |
| 11:A:226:U:O2'    | 11:A:229:G:H4'    | 2.21                     | 0.41              |
| 11:A:174:C:H3'    | 11:A:175:U:C6     | 2.55                     | 0.41              |
| 11:A:741:U:C3'    | 11:A:742:A:H5''   | 2.51                     | 0.41              |
| 21:O:89:HIS:HA    | 21:O:103:ASN:HD22 | 1.85                     | 0.41              |
| 11:A:1180:G:O2'   | 11:A:1247:A:N6    | 2.53                     | 0.41              |
| 9:8:127:ALA:HA    | 22:P:79:PRO:HD3   | 2.02                     | 0.41              |
| 11:A:648:A:O2'    | 11:A:782:G:H5''   | 2.20                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:P:223:LEU:HD23 | 22:P:223:LEU:HA   | 1.80                     | 0.41              |
| 4:3:91:LEU:HD23   | 4:3:91:LEU:HA     | 1.75                     | 0.41              |
| 8:7:74:ARG:HD3    | 8:7:74:ARG:HA     | 1.54                     | 0.41              |
| 11:A:772:A:H8     | 11:A:772:A:H5'    | 1.85                     | 0.41              |
| 11:A:781:A:C2     | 24:R:20:LEU:HG    | 2.55                     | 0.41              |
| 12:B:4:P5P:H2'    | 12:B:5:P5P:C8     | 2.50                     | 0.41              |
| 8:7:66:LYS:O      | 8:7:71:ARG:HG2    | 2.21                     | 0.41              |
| 28:V:63:PRO:HA    | 28:V:64:PRO:HD3   | 1.69                     | 0.41              |
| 11:A:251:G:N1     | 11:A:320:A:C2     | 2.88                     | 0.41              |
| 12:B:14:P5P:H5'2  | 12:B:15:P5P:OP2   | 2.20                     | 0.41              |
| 9:8:123:LEU:HD12  | 9:8:148:VAL:O     | 2.20                     | 0.41              |
| 11:A:1395:G:H2'   | 11:A:1396:U:O4'   | 2.20                     | 0.41              |
| 24:R:65:LEU:HA    | 24:R:65:LEU:HD23  | 1.91                     | 0.41              |
| 11:A:511:A:H61    | 11:A:512:A:N6     | 2.18                     | 0.41              |
| 21:O:51:TYR:CZ    | 21:O:78:ARG:HA    | 2.55                     | 0.41              |
| 11:A:1418:A:H5'   | 14:D:278:ARG:NH2  | 2.36                     | 0.41              |
| 11:A:255:U:C2'    | 11:A:256:A:H5'    | 2.50                     | 0.41              |
| 6:5:96:ASN:ND2    | 11:A:1039:A:O4'   | 2.52                     | 0.41              |
| 6:5:96:ASN:HD21   | 11:A:1038:A:H2'   | 1.85                     | 0.41              |
| 27:U:58:ARG:HG2   | 27:U:62:ARG:NH2   | 2.36                     | 0.41              |
| 24:R:153:LEU:HA   | 24:R:153:LEU:HD23 | 1.68                     | 0.41              |
| 4:3:110:LEU:HD23  | 4:3:110:LEU:HA    | 1.88                     | 0.41              |
| 1:0:107:ASN:OD1   | 1:0:108:PRO:HD2   | 2.20                     | 0.41              |
| 22:P:269:LEU:HA   | 22:P:269:LEU:HD23 | 1.91                     | 0.41              |
| 12:B:23:P5P:H2'   | 12:B:24:P5P:O4'   | 2.20                     | 0.41              |
| 16:F:71:GLY:H     | 16:F:74:GLN:HE21  | 1.69                     | 0.41              |
| 14:D:113:ARG:HB3  | 14:D:148:ARG:HH22 | 1.85                     | 0.41              |
| 11:A:386:A:C3'    | 11:A:387:A:H5''   | 2.50                     | 0.41              |
| 26:T:136:ILE:O    | 26:T:151:LEU:HA   | 2.21                     | 0.41              |
| 17:I:70:LYS:HA    | 17:I:71:PRO:HD3   | 1.82                     | 0.41              |
| 11:A:1240:U:O2'   | 11:A:1241:U:OP2   | 2.34                     | 0.41              |
| 16:F:195:LEU:HG   | 16:F:230:VAL:HG22 | 2.03                     | 0.41              |
| 2:1:88:GLY:C      | 2:1:89:HIS:HD2    | 2.24                     | 0.41              |
| 17:I:73:LEU:HD23  | 17:I:73:LEU:HA    | 1.84                     | 0.41              |
| 15:E:239:ARG:H    | 15:E:239:ARG:HG3  | 1.59                     | 0.41              |
| 15:E:206:VAL:HG11 | 15:E:289:VAL:HG13 | 2.03                     | 0.41              |
| 7:6:47:ASP:HB2    | 7:6:54:VAL:CG2    | 2.45                     | 0.41              |
| 12:B:9:P5P:H5'2   | 12:B:47:P5P:C1'   | 2.49                     | 0.41              |
| 20:N:27:PRO:HA    | 20:N:66:ALA:O     | 2.20                     | 0.41              |
| 3:2:100:LEU:HD22  | 3:2:144:LEU:CD1   | 2.51                     | 0.41              |
| 11:A:196:U:O3'    | 27:U:38:CYS:HB3   | 2.20                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:A:275:G:H5''   | 14:D:260:LYS:HD3  | 2.02                     | 0.41              |
| 15:E:195:ALA:HB3  | 15:E:281:ASN:HD22 | 1.86                     | 0.41              |
| 11:A:507:C:H2'    | 11:A:508:C:O4'    | 2.21                     | 0.41              |
| 15:E:279:LYS:HB2  | 15:E:330:GLU:OE1  | 2.20                     | 0.41              |
| 14:D:129:ALA:HB1  | 14:D:131:ARG:HE   | 1.85                     | 0.41              |
| 26:T:145:LEU:HA   | 26:T:145:LEU:HD12 | 1.84                     | 0.41              |
| 11:A:70:A:N3      | 11:A:70:A:H2'     | 2.36                     | 0.41              |
| 11:A:1312:U:HO2'  | 11:A:1313:U:H6    | 1.69                     | 0.41              |
| 25:S:126:GLU:OE2  | 25:S:160:ARG:HD3  | 2.20                     | 0.41              |
| 11:A:429:A:OP1    | 22:P:57:ARG:HD2   | 2.20                     | 0.41              |
| 12:B:63:Y5P:O5'   | 12:B:63:Y5P:H6    | 2.21                     | 0.41              |
| 18:J:188:ARG:O    | 18:J:192:ILE:HG13 | 2.20                     | 0.41              |
| 11:A:1074:A:H2'   | 11:A:1075:A:H8    | 1.82                     | 0.41              |
| 11:A:522:C:C5     | 11:A:530:A:H5''   | 2.54                     | 0.41              |
| 31:Y:58:CYS:HB2   | 31:Y:77:VAL:O     | 2.20                     | 0.41              |
| 11:A:1545:A:N7    | 15:E:178:ILE:HD12 | 2.36                     | 0.41              |
| 22:P:127:VAL:HG11 | 22:P:138:VAL:CG2  | 2.51                     | 0.41              |
| 15:E:54:SER:O     | 15:E:58:VAL:HG23  | 2.21                     | 0.41              |
| 18:J:132:LYS:O    | 18:J:136:GLU:HG3  | 2.21                     | 0.41              |
| 27:U:116:LEU:HD23 | 27:U:116:LEU:HA   | 1.75                     | 0.41              |
| 11:A:118:U:H2'    | 11:A:119:A:H5''   | 2.03                     | 0.41              |
| 9:8:103:LYS:NZ    | 11:A:76:G:OP2     | 2.53                     | 0.41              |
| 26:T:235:ARG:HA   | 26:T:236:PRO:HD3  | 1.78                     | 0.41              |
| 2:1:71:TYR:HA     | 2:1:72:PRO:HD2    | 1.94                     | 0.41              |
| 27:U:126:GLU:OE2  | 28:V:70:LEU:HD21  | 2.21                     | 0.41              |
| 11:A:137:A:C2     | 11:A:139:A:C4     | 3.09                     | 0.41              |
| 29:W:58:PRO:HA    | 29:W:59:PRO:HD3   | 1.88                     | 0.41              |
| 12:B:48:Y5P:HA    | 12:B:49:P5P:O5'   | 2.20                     | 0.41              |
| 11:A:844:C:C3'    | 11:A:845:U:H5''   | 2.51                     | 0.41              |
| 31:Y:146:VAL:HA   | 31:Y:152:ARG:O    | 2.21                     | 0.41              |
| 4:3:73:LYS:HA     | 11:A:471:U:OP1    | 2.20                     | 0.41              |
| 11:A:3:C:OP1      | 29:W:171:HIS:HE1  | 2.04                     | 0.41              |
| 15:E:285:VAL:HG12 | 15:E:286:ASN:N    | 2.33                     | 0.41              |
| 24:R:142:ASN:O    | 24:R:148:GLN:NE2  | 2.54                     | 0.41              |
| 27:U:94:GLN:HE22  | 27:U:145:VAL:HG13 | 1.85                     | 0.41              |
| 11:A:1490:C:N3    | 24:R:15:PHE:HD2   | 2.19                     | 0.41              |
| 22:P:68:GLU:HG3   | 22:P:73:PRO:HA    | 2.02                     | 0.41              |
| 9:8:118:HIS:CD2   | 9:8:169:ARG:HH11  | 2.39                     | 0.41              |
| 7:6:22:SER:HB3    | 7:6:56:PHE:CZ     | 2.56                     | 0.41              |
| 29:W:157:HIS:HB2  | 29:W:161:ARG:O    | 2.21                     | 0.41              |
| 2:1:128:THR:HG22  | 2:1:129:MET:N     | 2.36                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:A:492:U:H2'    | 11:A:493:A:H5''   | 2.02                     | 0.40              |
| 11:A:113:G:N2     | 11:A:116:A:O2'    | 2.54                     | 0.40              |
| 11:A:1210:U:H5'   | 11:A:1211:A:OP2   | 2.21                     | 0.40              |
| 11:A:168:U:H5''   | 11:A:169:U:OP1    | 2.21                     | 0.40              |
| 6:5:160:TYR:CD2   | 6:5:181:ARG:HB2   | 2.56                     | 0.40              |
| 7:6:19:LYS:HE3    | 7:6:28:PHE:CD1    | 2.56                     | 0.40              |
| 23:Q:92:LEU:HD23  | 23:Q:92:LEU:HA    | 1.75                     | 0.40              |
| 11:A:476:A:H3'    | 11:A:477:G:H5''   | 2.03                     | 0.40              |
| 24:R:131:LEU:HD23 | 24:R:131:LEU:HA   | 1.94                     | 0.40              |
| 11:A:241:G:H5'    | 16:F:139:GLY:N    | 2.35                     | 0.40              |
| 19:K:54:ASN:HB3   | 19:K:58:LYS:CE    | 2.52                     | 0.40              |
| 3:2:100:LEU:HD23  | 3:2:100:LEU:HA    | 1.89                     | 0.40              |
| 18:J:46:LYS:O     | 18:J:50:VAL:HG23  | 2.21                     | 0.40              |
| 20:N:90:VAL:CG1   | 20:N:94:GLN:HB2   | 2.51                     | 0.40              |
| 11:A:147:A:OP2    | 11:A:147:A:H8     | 2.04                     | 0.40              |
| 24:R:28:LEU:HA    | 24:R:28:LEU:HD23  | 1.94                     | 0.40              |
| 8:7:83:LEU:HD23   | 8:7:83:LEU:HA     | 1.87                     | 0.40              |
| 25:S:86:THR:O     | 25:S:120:ARG:NH1  | 2.53                     | 0.40              |
| 15:E:341:GLY:CA   | 26:T:105:ILE:HD11 | 2.47                     | 0.40              |
| 14:D:123:PHE:O    | 14:D:165:LEU:HD12 | 2.20                     | 0.40              |
| 26:T:74:ARG:HD3   | 26:T:283:TRP:NE1  | 2.36                     | 0.40              |
| 11:A:350:A:H5'    | 11:A:351:G:OP2    | 2.20                     | 0.40              |
| 4:3:88:MET:HE3    | 11:A:416:G:H21    | 1.86                     | 0.40              |
| 11:A:197:U:H2'    | 11:A:198:A:C8     | 2.56                     | 0.40              |
| 9:8:118:HIS:CG    | 9:8:169:ARG:HD3   | 2.56                     | 0.40              |
| 20:N:10:GLN:HE21  | 29:W:202:ARG:HA   | 1.86                     | 0.40              |
| 14:D:139:ASP:OD2  | 14:D:250:ASN:HB2  | 2.20                     | 0.40              |
| 11:A:560:A:H3'    | 11:A:560:A:N3     | 2.36                     | 0.40              |
| 11:A:845:U:H2'    | 11:A:846:C:O4'    | 2.21                     | 0.40              |
| 11:A:504:A:H1'    | 11:A:513:A:C8     | 2.57                     | 0.40              |
| 23:Q:172:VAL:H    | 23:Q:172:VAL:HG23 | 1.68                     | 0.40              |
| 11:A:520:A:H5''   | 11:A:521:U:OP2    | 2.21                     | 0.40              |
| 11:A:936:U:C4'    | 11:A:937:U:H3'    | 2.52                     | 0.40              |
| 14:D:290:LEU:HD12 | 14:D:291:PRO:HD2  | 2.02                     | 0.40              |
| 2:1:79:LEU:HG     | 2:1:125:VAL:HG11  | 2.03                     | 0.40              |
| 18:J:113:ARG:HG2  | 18:J:123:MET:SD   | 2.62                     | 0.40              |
| 15:E:293:LYS:HE2  | 15:E:293:LYS:HB3  | 1.72                     | 0.40              |
| 11:A:503:U:H5''   | 19:K:86:THR:HG23  | 2.03                     | 0.40              |
| 18:J:176:LEU:HB3  | 18:J:188:ARG:HH11 | 1.87                     | 0.40              |
| 26:T:240:ILE:HG21 | 26:T:243:ILE:HG12 | 2.02                     | 0.40              |
| 2:1:23:ARG:HD3    | 2:1:219:GLU:OE2   | 2.20                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:A:1238:A:O2'   | 11:A:1239:U:OP2   | 2.36                     | 0.40              |
| 11:A:673:U:H5''   | 30:X:78:ARG:HB2   | 2.04                     | 0.40              |
| 31:Y:98:VAL:CG2   | 31:Y:109:ILE:HD12 | 2.52                     | 0.40              |
| 11:A:420:U:H2'    | 11:A:421:U:H6     | 1.86                     | 0.40              |
| 26:T:112:TYR:CE2  | 26:T:181:LYS:HE2  | 2.57                     | 0.40              |
| 21:O:58:ILE:HD11  | 21:O:76:ALA:HB2   | 2.02                     | 0.40              |
| 12:B:11:Y5P:H4A   | 12:B:12:Y5P:H4    | 2.04                     | 0.40              |
| 29:W:96:SER:HB3   | 29:W:181:PRO:HG3  | 2.03                     | 0.40              |
| 14:D:247:ARG:NH1  | 14:D:251:VAL:HG11 | 2.36                     | 0.40              |
| 14:D:258:ILE:HG23 | 14:D:263:ARG:CB   | 2.51                     | 0.40              |
| 28:V:170:SER:HB2  | 28:V:194:GLN:CD   | 2.42                     | 0.40              |
| 19:K:111:LEU:HD11 | 19:K:156:VAL:HG23 | 2.03                     | 0.40              |
| 20:N:138:LEU:HA   | 20:N:138:LEU:HD23 | 1.89                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1   | 0     | 112/148 (76%) | 110 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 2   | 1     | 242/256 (94%) | 235 (97%) | 7 (3%)  | 0        | 100         | 100 |
| 3   | 2     | 176/252 (70%) | 167 (95%) | 9 (5%)  | 0        | 100         | 100 |
| 4   | 3     | 116/161 (72%) | 113 (97%) | 3 (3%)  | 0        | 100         | 100 |
| 5   | 4     | 43/126 (34%)  | 42 (98%)  | 1 (2%)  | 0        | 100         | 100 |
| 6   | 5     | 108/188 (57%) | 107 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 7   | 6     | 46/65 (71%)   | 44 (96%)  | 2 (4%)  | 0        | 100         | 100 |
| 8   | 7     | 44/95 (46%)   | 44 (100%) | 0       | 0        | 100         | 100 |
| 9   | 8     | 93/188 (50%)  | 91 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 10  | 9     | 36/100 (36%)  | 36 (100%) | 0       | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 14  | D     | 238/306 (78%)   | 230 (97%)  | 8 (3%)   | 0        | 100         | 100 |
| 15  | E     | 305/348 (88%)   | 279 (92%)  | 24 (8%)  | 2 (1%)   | 26          | 70  |
| 16  | F     | 248/294 (84%)   | 237 (96%)  | 10 (4%)  | 1 (0%)   | 39          | 79  |
| 17  | I     | 96/268 (36%)    | 87 (91%)   | 9 (9%)   | 0        | 100         | 100 |
| 18  | J     | 166/262 (63%)   | 158 (95%)  | 8 (5%)   | 0        | 100         | 100 |
| 19  | K     | 140/192 (73%)   | 133 (95%)  | 7 (5%)   | 0        | 100         | 100 |
| 20  | N     | 175/178 (98%)   | 171 (98%)  | 4 (2%)   | 0        | 100         | 100 |
| 21  | O     | 113/145 (78%)   | 109 (96%)  | 4 (4%)   | 0        | 100         | 100 |
| 22  | P     | 286/296 (97%)   | 275 (96%)  | 11 (4%)  | 0        | 100         | 100 |
| 23  | Q     | 219/251 (87%)   | 217 (99%)  | 2 (1%)   | 0        | 100         | 100 |
| 24  | R     | 151/169 (89%)   | 148 (98%)  | 3 (2%)   | 0        | 100         | 100 |
| 25  | S     | 141/180 (78%)   | 128 (91%)  | 12 (8%)  | 1 (1%)   | 26          | 70  |
| 26  | T     | 222/292 (76%)   | 215 (97%)  | 6 (3%)   | 1 (0%)   | 34          | 75  |
| 27  | U     | 138/149 (93%)   | 136 (99%)  | 2 (1%)   | 0        | 100         | 100 |
| 28  | V     | 153/209 (73%)   | 148 (97%)  | 5 (3%)   | 0        | 100         | 100 |
| 29  | W     | 164/210 (78%)   | 159 (97%)  | 5 (3%)   | 0        | 100         | 100 |
| 30  | X     | 130/150 (87%)   | 125 (96%)  | 5 (4%)   | 0        | 100         | 100 |
| 31  | Y     | 202/216 (94%)   | 191 (95%)  | 11 (5%)  | 0        | 100         | 100 |
| All | All   | 4303/5694 (76%) | 4135 (96%) | 163 (4%) | 5 (0%)   | 59          | 89  |

All (5) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 15  | E     | 202 | GLN  |
| 15  | E     | 317 | PRO  |
| 26  | T     | 270 | MET  |
| 16  | F     | 291 | CYS  |
| 25  | S     | 45  | ALA  |

### 5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1   | 0     | 92/115 (80%)    | 82 (89%)   | 10 (11%) | 8           | 34 |
| 2   | 1     | 219/229 (96%)   | 209 (95%)  | 10 (5%)  | 33          | 72 |
| 3   | 2     | 164/228 (72%)   | 160 (98%)  | 4 (2%)   | 57          | 85 |
| 4   | 3     | 110/147 (75%)   | 107 (97%)  | 3 (3%)   | 52          | 83 |
| 5   | 4     | 42/114 (37%)    | 38 (90%)   | 4 (10%)  | 11          | 41 |
| 6   | 5     | 99/163 (61%)    | 96 (97%)   | 3 (3%)   | 48          | 81 |
| 7   | 6     | 45/60 (75%)     | 41 (91%)   | 4 (9%)   | 12          | 45 |
| 8   | 7     | 41/78 (53%)     | 36 (88%)   | 5 (12%)  | 6           | 28 |
| 9   | 8     | 87/162 (54%)    | 75 (86%)   | 12 (14%) | 4           | 23 |
| 10  | 9     | 36/77 (47%)     | 34 (94%)   | 2 (6%)   | 26          | 66 |
| 14  | D     | 193/248 (78%)   | 186 (96%)  | 7 (4%)   | 42          | 78 |
| 15  | E     | 263/290 (91%)   | 246 (94%)  | 17 (6%)  | 21          | 61 |
| 16  | F     | 217/251 (86%)   | 200 (92%)  | 17 (8%)  | 16          | 52 |
| 17  | I     | 88/228 (39%)    | 84 (96%)   | 4 (4%)   | 34          | 73 |
| 18  | J     | 154/230 (67%)   | 145 (94%)  | 9 (6%)   | 25          | 65 |
| 19  | K     | 115/151 (76%)   | 107 (93%)  | 8 (7%)   | 19          | 58 |
| 20  | N     | 156/157 (99%)   | 148 (95%)  | 8 (5%)   | 29          | 69 |
| 21  | O     | 99/123 (80%)    | 91 (92%)   | 8 (8%)   | 15          | 51 |
| 22  | P     | 245/249 (98%)   | 231 (94%)  | 14 (6%)  | 25          | 65 |
| 23  | Q     | 189/210 (90%)   | 179 (95%)  | 10 (5%)  | 28          | 67 |
| 24  | R     | 132/143 (92%)   | 122 (92%)  | 10 (8%)  | 16          | 54 |
| 25  | S     | 123/153 (80%)   | 118 (96%)  | 5 (4%)   | 37          | 75 |
| 26  | T     | 206/258 (80%)   | 197 (96%)  | 9 (4%)   | 35          | 73 |
| 27  | U     | 118/127 (93%)   | 109 (92%)  | 9 (8%)   | 16          | 54 |
| 28  | V     | 136/178 (76%)   | 127 (93%)  | 9 (7%)   | 21          | 61 |
| 29  | W     | 144/180 (80%)   | 135 (94%)  | 9 (6%)   | 22          | 62 |
| 30  | X     | 119/134 (89%)   | 110 (92%)  | 9 (8%)   | 16          | 54 |
| 31  | Y     | 183/192 (95%)   | 170 (93%)  | 13 (7%)  | 18          | 58 |
| All | All   | 3815/4875 (78%) | 3583 (94%) | 232 (6%) | 28          | 63 |

All (232) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 0     | 45  | LYS  |
| 1   | 0     | 46  | SER  |
| 1   | 0     | 50  | ARG  |
| 1   | 0     | 57  | GLU  |
| 1   | 0     | 71  | ARG  |
| 1   | 0     | 75  | TRP  |
| 1   | 0     | 88  | CYS  |
| 1   | 0     | 94  | GLU  |
| 1   | 0     | 117 | VAL  |
| 1   | 0     | 126 | LEU  |
| 2   | 1     | 61  | ARG  |
| 2   | 1     | 69  | VAL  |
| 2   | 1     | 90  | ARG  |
| 2   | 1     | 101 | VAL  |
| 2   | 1     | 104 | VAL  |
| 2   | 1     | 120 | ASP  |
| 2   | 1     | 159 | MET  |
| 2   | 1     | 173 | ASP  |
| 2   | 1     | 177 | HIS  |
| 2   | 1     | 179 | ASP  |
| 3   | 2     | 83  | SER  |
| 3   | 2     | 153 | ASP  |
| 3   | 2     | 156 | ARG  |
| 3   | 2     | 228 | LEU  |
| 4   | 3     | 40  | ARG  |
| 4   | 3     | 88  | MET  |
| 4   | 3     | 147 | VAL  |
| 5   | 4     | 38  | ARG  |
| 5   | 4     | 42  | THR  |
| 5   | 4     | 43  | ARG  |
| 5   | 4     | 60  | GLN  |
| 6   | 5     | 92  | CYS  |
| 6   | 5     | 156 | THR  |
| 6   | 5     | 186 | THR  |
| 7   | 6     | 18  | VAL  |
| 7   | 6     | 32  | THR  |
| 7   | 6     | 42  | THR  |
| 7   | 6     | 54  | VAL  |
| 8   | 7     | 65  | HIS  |
| 8   | 7     | 74  | ARG  |
| 8   | 7     | 77  | THR  |
| 8   | 7     | 94  | SER  |
| 8   | 7     | 95  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9   | 8     | 98  | SER  |
| 9   | 8     | 106 | THR  |
| 9   | 8     | 111 | ILE  |
| 9   | 8     | 113 | ARG  |
| 9   | 8     | 116 | ARG  |
| 9   | 8     | 124 | ARG  |
| 9   | 8     | 148 | VAL  |
| 9   | 8     | 150 | CYS  |
| 9   | 8     | 162 | THR  |
| 9   | 8     | 163 | THR  |
| 9   | 8     | 169 | ARG  |
| 9   | 8     | 183 | ARG  |
| 10  | 9     | 75  | ASP  |
| 10  | 9     | 100 | MET  |
| 14  | D     | 62  | THR  |
| 14  | D     | 105 | ARG  |
| 14  | D     | 111 | ARG  |
| 14  | D     | 148 | ARG  |
| 14  | D     | 179 | GLU  |
| 14  | D     | 256 | ARG  |
| 14  | D     | 278 | ARG  |
| 15  | E     | 94  | SER  |
| 15  | E     | 96  | ARG  |
| 15  | E     | 102 | LEU  |
| 15  | E     | 118 | VAL  |
| 15  | E     | 127 | CYS  |
| 15  | E     | 153 | SER  |
| 15  | E     | 189 | PRO  |
| 15  | E     | 220 | ARG  |
| 15  | E     | 227 | GLN  |
| 15  | E     | 236 | THR  |
| 15  | E     | 239 | ARG  |
| 15  | E     | 251 | VAL  |
| 15  | E     | 273 | VAL  |
| 15  | E     | 288 | SER  |
| 15  | E     | 295 | CYS  |
| 15  | E     | 296 | LEU  |
| 15  | E     | 344 | SER  |
| 16  | F     | 68  | SER  |
| 16  | F     | 76  | ARG  |
| 16  | F     | 79  | LEU  |
| 16  | F     | 111 | TYR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 16  | F     | 114 | THR  |
| 16  | F     | 125 | ARG  |
| 16  | F     | 143 | SER  |
| 16  | F     | 147 | ARG  |
| 16  | F     | 164 | MET  |
| 16  | F     | 174 | LEU  |
| 16  | F     | 190 | VAL  |
| 16  | F     | 203 | LEU  |
| 16  | F     | 226 | MET  |
| 16  | F     | 234 | THR  |
| 16  | F     | 239 | THR  |
| 16  | F     | 241 | ASN  |
| 16  | F     | 284 | TYR  |
| 17  | I     | 64  | LEU  |
| 17  | I     | 79  | VAL  |
| 17  | I     | 83  | VAL  |
| 17  | I     | 108 | ARG  |
| 18  | J     | 35  | ARG  |
| 18  | J     | 38  | ARG  |
| 18  | J     | 61  | ASN  |
| 18  | J     | 63  | ARG  |
| 18  | J     | 65  | LEU  |
| 18  | J     | 76  | THR  |
| 18  | J     | 116 | LEU  |
| 18  | J     | 150 | HIS  |
| 18  | J     | 183 | ASP  |
| 19  | K     | 64  | ILE  |
| 19  | K     | 66  | LEU  |
| 19  | K     | 70  | ILE  |
| 19  | K     | 80  | ILE  |
| 19  | K     | 97  | ILE  |
| 19  | K     | 113 | THR  |
| 19  | K     | 128 | ASP  |
| 19  | K     | 135 | VAL  |
| 20  | N     | 2   | SER  |
| 20  | N     | 25  | MET  |
| 20  | N     | 36  | SER  |
| 20  | N     | 67  | PHE  |
| 20  | N     | 78  | SER  |
| 20  | N     | 104 | VAL  |
| 20  | N     | 118 | ARG  |
| 20  | N     | 177 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 21  | O     | 33  | GLN  |
| 21  | O     | 48  | THR  |
| 21  | O     | 73  | ILE  |
| 21  | O     | 77  | ILE  |
| 21  | O     | 91  | MET  |
| 21  | O     | 95  | ARG  |
| 21  | O     | 121 | THR  |
| 21  | O     | 138 | LEU  |
| 22  | P     | 30  | ASN  |
| 22  | P     | 43  | ARG  |
| 22  | P     | 44  | ARG  |
| 22  | P     | 47  | ARG  |
| 22  | P     | 61  | THR  |
| 22  | P     | 62  | ARG  |
| 22  | P     | 64  | ARG  |
| 22  | P     | 65  | LEU  |
| 22  | P     | 88  | SER  |
| 22  | P     | 130 | GLN  |
| 22  | P     | 141 | VAL  |
| 22  | P     | 215 | THR  |
| 22  | P     | 284 | LYS  |
| 22  | P     | 286 | THR  |
| 23  | Q     | 62  | VAL  |
| 23  | Q     | 86  | ARG  |
| 23  | Q     | 96  | TYR  |
| 23  | Q     | 104 | MET  |
| 23  | Q     | 109 | ILE  |
| 23  | Q     | 110 | ASN  |
| 23  | Q     | 163 | MET  |
| 23  | Q     | 209 | ASN  |
| 23  | Q     | 226 | ILE  |
| 23  | Q     | 234 | ASP  |
| 24  | R     | 9   | ILE  |
| 24  | R     | 14  | VAL  |
| 24  | R     | 16  | ARG  |
| 24  | R     | 25  | ARG  |
| 24  | R     | 50  | ASP  |
| 24  | R     | 61  | ASP  |
| 24  | R     | 116 | GLN  |
| 24  | R     | 118 | ARG  |
| 24  | R     | 123 | VAL  |
| 24  | R     | 142 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 25  | S     | 44  | VAL  |
| 25  | S     | 66  | ARG  |
| 25  | S     | 70  | THR  |
| 25  | S     | 71  | VAL  |
| 25  | S     | 80  | ARG  |
| 26  | T     | 115 | SER  |
| 26  | T     | 134 | LEU  |
| 26  | T     | 138 | ILE  |
| 26  | T     | 187 | LEU  |
| 26  | T     | 208 | THR  |
| 26  | T     | 254 | MET  |
| 26  | T     | 270 | MET  |
| 26  | T     | 275 | THR  |
| 26  | T     | 276 | SER  |
| 27  | U     | 10  | LEU  |
| 27  | U     | 15  | THR  |
| 27  | U     | 24  | VAL  |
| 27  | U     | 46  | VAL  |
| 27  | U     | 53  | CYS  |
| 27  | U     | 55  | ARG  |
| 27  | U     | 76  | SER  |
| 27  | U     | 93  | CYS  |
| 27  | U     | 102 | LEU  |
| 28  | V     | 65  | TRP  |
| 28  | V     | 128 | CYS  |
| 28  | V     | 131 | ARG  |
| 28  | V     | 152 | LEU  |
| 28  | V     | 153 | LEU  |
| 28  | V     | 164 | VAL  |
| 28  | V     | 170 | SER  |
| 28  | V     | 186 | ARG  |
| 28  | V     | 199 | ILE  |
| 29  | W     | 60  | GLN  |
| 29  | W     | 67  | ARG  |
| 29  | W     | 75  | ARG  |
| 29  | W     | 77  | GLN  |
| 29  | W     | 80  | TYR  |
| 29  | W     | 144 | THR  |
| 29  | W     | 151 | LEU  |
| 29  | W     | 199 | GLN  |
| 29  | W     | 207 | THR  |
| 30  | X     | 18  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 30  | X     | 40  | VAL  |
| 30  | X     | 49  | THR  |
| 30  | X     | 57  | LEU  |
| 30  | X     | 77  | ASN  |
| 30  | X     | 97  | VAL  |
| 30  | X     | 141 | ARG  |
| 30  | X     | 148 | PHE  |
| 30  | X     | 150 | LEU  |
| 31  | Y     | 78  | GLN  |
| 31  | Y     | 79  | VAL  |
| 31  | Y     | 105 | ARG  |
| 31  | Y     | 111 | SER  |
| 31  | Y     | 131 | THR  |
| 31  | Y     | 137 | PHE  |
| 31  | Y     | 138 | THR  |
| 31  | Y     | 145 | ARG  |
| 31  | Y     | 149 | ARG  |
| 31  | Y     | 161 | ARG  |
| 31  | Y     | 166 | VAL  |
| 31  | Y     | 193 | THR  |
| 31  | Y     | 196 | GLU  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 0     | 41  | ASN  |
| 1   | 0     | 59  | HIS  |
| 1   | 0     | 65  | ASN  |
| 1   | 0     | 76  | HIS  |
| 2   | 1     | 27  | HIS  |
| 2   | 1     | 42  | HIS  |
| 3   | 2     | 97  | ASN  |
| 3   | 2     | 197 | ASN  |
| 4   | 3     | 67  | HIS  |
| 5   | 4     | 37  | ASN  |
| 6   | 5     | 83  | ASN  |
| 6   | 5     | 170 | GLN  |
| 7   | 6     | 23  | GLN  |
| 8   | 7     | 95  | HIS  |
| 9   | 8     | 118 | HIS  |
| 10  | 9     | 92  | ASN  |
| 14  | D     | 116 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 14  | D     | 183 | HIS  |
| 14  | D     | 195 | ASN  |
| 14  | D     | 196 | ASN  |
| 14  | D     | 272 | ASN  |
| 15  | E     | 128 | HIS  |
| 15  | E     | 281 | ASN  |
| 15  | E     | 292 | HIS  |
| 16  | F     | 74  | GLN  |
| 16  | F     | 83  | HIS  |
| 16  | F     | 103 | GLN  |
| 16  | F     | 105 | ASN  |
| 16  | F     | 153 | HIS  |
| 16  | F     | 241 | ASN  |
| 16  | F     | 249 | ASN  |
| 16  | F     | 276 | HIS  |
| 17  | I     | 93  | ASN  |
| 17  | I     | 136 | ASN  |
| 18  | J     | 41  | HIS  |
| 19  | K     | 103 | HIS  |
| 19  | K     | 126 | GLN  |
| 21  | O     | 89  | HIS  |
| 21  | O     | 103 | ASN  |
| 22  | P     | 53  | HIS  |
| 22  | P     | 71  | GLN  |
| 22  | P     | 84  | ASN  |
| 22  | P     | 87  | HIS  |
| 22  | P     | 91  | HIS  |
| 22  | P     | 130 | GLN  |
| 22  | P     | 170 | ASN  |
| 23  | Q     | 98  | HIS  |
| 23  | Q     | 110 | ASN  |
| 23  | Q     | 209 | ASN  |
| 23  | Q     | 210 | GLN  |
| 24  | R     | 39  | HIS  |
| 24  | R     | 112 | ASN  |
| 24  | R     | 142 | ASN  |
| 24  | R     | 147 | ASN  |
| 24  | R     | 148 | GLN  |
| 25  | S     | 96  | HIS  |
| 26  | T     | 132 | GLN  |
| 26  | T     | 139 | GLN  |
| 26  | T     | 158 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 27  | U     | 89  | ASN  |
| 27  | U     | 94  | GLN  |
| 28  | V     | 80  | HIS  |
| 28  | V     | 104 | HIS  |
| 28  | V     | 109 | GLN  |
| 29  | W     | 130 | HIS  |
| 29  | W     | 171 | HIS  |
| 29  | W     | 199 | GLN  |
| 29  | W     | 203 | ASN  |
| 30  | X     | 14  | ASN  |
| 30  | X     | 41  | GLN  |
| 30  | X     | 73  | GLN  |
| 30  | X     | 77  | ASN  |
| 30  | X     | 135 | HIS  |
| 31  | Y     | 78  | GLN  |
| 31  | Y     | 117 | HIS  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 11  | A     | 1508/1570 (96%) | 726 (48%)         | 29 (1%)         |
| 12  | B     | 0/62            | -                 | -               |
| 13  | C     | 2/3 (66%)       | 2 (100%)          | 0               |
| 13  | Z     | 2/3 (66%)       | 0                 | 0               |
| All | All   | 1512/1638 (92%) | 728 (48%)         | 29 (1%)         |

All (728) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11  | A     | 4   | A    |
| 11  | A     | 5   | A    |
| 11  | A     | 7   | G    |
| 11  | A     | 11  | G    |
| 11  | A     | 12  | C    |
| 11  | A     | 16  | A    |
| 11  | A     | 27  | A    |
| 11  | A     | 30  | U    |
| 11  | A     | 31  | A    |
| 11  | A     | 32  | C    |
| 11  | A     | 36  | A    |
| 11  | A     | 37  | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11  | A     | 39  | A    |
| 11  | A     | 40  | C    |
| 11  | A     | 41  | A    |
| 11  | A     | 42  | C    |
| 11  | A     | 43  | C    |
| 11  | A     | 44  | A    |
| 11  | A     | 45  | A    |
| 11  | A     | 46  | A    |
| 11  | A     | 49  | A    |
| 11  | A     | 50  | A    |
| 11  | A     | 56  | A    |
| 11  | A     | 58  | C    |
| 11  | A     | 59  | A    |
| 11  | A     | 60  | U    |
| 11  | A     | 63  | A    |
| 11  | A     | 64  | C    |
| 11  | A     | 66  | U    |
| 11  | A     | 67  | A    |
| 11  | A     | 68  | A    |
| 11  | A     | 69  | C    |
| 11  | A     | 71  | U    |
| 11  | A     | 72  | U    |
| 11  | A     | 82  | G    |
| 11  | A     | 83  | A    |
| 11  | A     | 84  | G    |
| 11  | A     | 96  | U    |
| 11  | A     | 97  | A    |
| 11  | A     | 98  | U    |
| 11  | A     | 99  | C    |
| 11  | A     | 100 | C    |
| 11  | A     | 101 | U    |
| 11  | A     | 102 | G    |
| 11  | A     | 104 | C    |
| 11  | A     | 105 | G    |
| 11  | A     | 106 | C    |
| 11  | A     | 107 | U    |
| 11  | A     | 108 | A    |
| 11  | A     | 109 | U    |
| 11  | A     | 110 | A    |
| 11  | A     | 112 | A    |
| 11  | A     | 113 | G    |
| 11  | A     | 114 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11  | A     | 115 | U    |
| 11  | A     | 116 | A    |
| 11  | A     | 117 | G    |
| 11  | A     | 119 | A    |
| 11  | A     | 122 | G    |
| 11  | A     | 123 | U    |
| 11  | A     | 124 | A    |
| 11  | A     | 128 | A    |
| 11  | A     | 130 | A    |
| 11  | A     | 131 | G    |
| 11  | A     | 132 | A    |
| 11  | A     | 135 | A    |
| 11  | A     | 136 | A    |
| 11  | A     | 138 | G    |
| 11  | A     | 139 | A    |
| 11  | A     | 140 | A    |
| 11  | A     | 147 | A    |
| 11  | A     | 148 | A    |
| 11  | A     | 155 | A    |
| 11  | A     | 156 | A    |
| 11  | A     | 157 | A    |
| 11  | A     | 158 | A    |
| 11  | A     | 159 | A    |
| 11  | A     | 160 | A    |
| 11  | A     | 161 | G    |
| 11  | A     | 162 | C    |
| 11  | A     | 163 | A    |
| 11  | A     | 164 | A    |
| 11  | A     | 167 | A    |
| 11  | A     | 168 | U    |
| 11  | A     | 169 | U    |
| 11  | A     | 171 | C    |
| 11  | A     | 172 | C    |
| 11  | A     | 175 | U    |
| 11  | A     | 177 | C    |
| 11  | A     | 178 | U    |
| 11  | A     | 179 | A    |
| 11  | A     | 187 | C    |
| 11  | A     | 189 | U    |
| 11  | A     | 191 | A    |
| 11  | A     | 203 | G    |
| 11  | A     | 204 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11  | A     | 206 | A    |
| 11  | A     | 207 | A    |
| 11  | A     | 213 | A    |
| 11  | A     | 216 | A    |
| 11  | A     | 217 | A    |
| 11  | A     | 218 | A    |
| 11  | A     | 222 | A    |
| 11  | A     | 224 | C    |
| 11  | A     | 227 | U    |
| 11  | A     | 228 | A    |
| 11  | A     | 229 | G    |
| 11  | A     | 236 | A    |
| 11  | A     | 237 | C    |
| 11  | A     | 238 | C    |
| 11  | A     | 241 | G    |
| 11  | A     | 242 | A    |
| 11  | A     | 243 | A    |
| 11  | A     | 253 | G    |
| 11  | A     | 256 | A    |
| 11  | A     | 259 | C    |
| 11  | A     | 262 | G    |
| 11  | A     | 271 | A    |
| 11  | A     | 272 | A    |
| 11  | A     | 273 | A    |
| 11  | A     | 274 | A    |
| 11  | A     | 275 | G    |
| 11  | A     | 276 | A    |
| 11  | A     | 277 | A    |
| 11  | A     | 280 | A    |
| 11  | A     | 281 | A    |
| 11  | A     | 283 | U    |
| 11  | A     | 284 | C    |
| 11  | A     | 286 | U    |
| 11  | A     | 293 | G    |
| 11  | A     | 294 | G    |
| 11  | A     | 296 | A    |
| 11  | A     | 297 | A    |
| 11  | A     | 300 | U    |
| 11  | A     | 304 | G    |
| 11  | A     | 307 | A    |
| 11  | A     | 308 | A    |
| 11  | A     | 310 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11  | A     | 311 | C    |
| 11  | A     | 312 | U    |
| 11  | A     | 317 | G    |
| 11  | A     | 321 | G    |
| 11  | A     | 322 | A    |
| 11  | A     | 323 | G    |
| 11  | A     | 328 | A    |
| 11  | A     | 329 | A    |
| 11  | A     | 330 | A    |
| 11  | A     | 331 | G    |
| 11  | A     | 332 | C    |
| 11  | A     | 335 | A    |
| 11  | A     | 336 | A    |
| 11  | A     | 337 | C    |
| 11  | A     | 338 | G    |
| 11  | A     | 339 | A    |
| 11  | A     | 347 | G    |
| 11  | A     | 348 | A    |
| 11  | A     | 351 | G    |
| 11  | A     | 352 | C    |
| 11  | A     | 356 | U    |
| 11  | A     | 357 | U    |
| 11  | A     | 358 | G    |
| 11  | A     | 362 | G    |
| 11  | A     | 364 | G    |
| 11  | A     | 365 | A    |
| 11  | A     | 367 | A    |
| 11  | A     | 368 | G    |
| 11  | A     | 369 | A    |
| 11  | A     | 370 | A    |
| 11  | A     | 372 | U    |
| 11  | A     | 373 | U    |
| 11  | A     | 375 | A    |
| 11  | A     | 382 | C    |
| 11  | A     | 387 | A    |
| 11  | A     | 388 | A    |
| 11  | A     | 389 | A    |
| 11  | A     | 390 | A    |
| 11  | A     | 391 | U    |
| 11  | A     | 393 | C    |
| 11  | A     | 396 | C    |
| 11  | A     | 397 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11  | A     | 398 | A    |
| 11  | A     | 401 | A    |
| 11  | A     | 403 | C    |
| 11  | A     | 404 | C    |
| 11  | A     | 406 | A    |
| 11  | A     | 408 | A    |
| 11  | A     | 413 | A    |
| 11  | A     | 416 | G    |
| 11  | A     | 417 | U    |
| 11  | A     | 422 | U    |
| 11  | A     | 426 | G    |
| 11  | A     | 427 | A    |
| 11  | A     | 428 | G    |
| 11  | A     | 432 | G    |
| 11  | A     | 439 | A    |
| 11  | A     | 441 | G    |
| 11  | A     | 444 | A    |
| 11  | A     | 445 | C    |
| 11  | A     | 447 | G    |
| 11  | A     | 448 | C    |
| 11  | A     | 454 | A    |
| 11  | A     | 458 | A    |
| 11  | A     | 459 | C    |
| 11  | A     | 461 | G    |
| 11  | A     | 463 | U    |
| 11  | A     | 464 | A    |
| 11  | A     | 465 | C    |
| 11  | A     | 467 | A    |
| 11  | A     | 472 | G    |
| 11  | A     | 473 | A    |
| 11  | A     | 474 | C    |
| 11  | A     | 475 | U    |
| 11  | A     | 476 | A    |
| 11  | A     | 477 | G    |
| 11  | A     | 478 | A    |
| 11  | A     | 479 | G    |
| 11  | A     | 482 | U    |
| 11  | A     | 486 | U    |
| 11  | A     | 487 | C    |
| 11  | A     | 488 | U    |
| 11  | A     | 490 | A    |
| 11  | A     | 491 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11  | A     | 492 | U    |
| 11  | A     | 493 | A    |
| 11  | A     | 495 | U    |
| 11  | A     | 497 | C    |
| 11  | A     | 498 | C    |
| 11  | A     | 499 | A    |
| 11  | A     | 500 | U    |
| 11  | A     | 501 | A    |
| 11  | A     | 502 | G    |
| 11  | A     | 503 | U    |
| 11  | A     | 504 | A    |
| 11  | A     | 505 | G    |
| 11  | A     | 508 | C    |
| 11  | A     | 509 | U    |
| 11  | A     | 510 | A    |
| 11  | A     | 513 | A    |
| 11  | A     | 514 | G    |
| 11  | A     | 515 | C    |
| 11  | A     | 518 | C    |
| 11  | A     | 519 | C    |
| 11  | A     | 521 | U    |
| 11  | A     | 522 | C    |
| 11  | A     | 523 | A    |
| 11  | A     | 524 | A    |
| 11  | A     | 525 | U    |
| 11  | A     | 526 | U    |
| 11  | A     | 527 | G    |
| 11  | A     | 528 | A    |
| 11  | A     | 529 | G    |
| 11  | A     | 530 | A    |
| 11  | A     | 532 | A    |
| 11  | A     | 533 | G    |
| 11  | A     | 534 | C    |
| 11  | A     | 536 | U    |
| 11  | A     | 538 | A    |
| 11  | A     | 539 | A    |
| 11  | A     | 542 | C    |
| 11  | A     | 543 | U    |
| 11  | A     | 545 | A    |
| 11  | A     | 546 | A    |
| 11  | A     | 548 | A    |
| 11  | A     | 550 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11  | A     | 551 | U    |
| 11  | A     | 552 | U    |
| 11  | A     | 553 | C    |
| 11  | A     | 554 | A    |
| 11  | A     | 555 | C    |
| 11  | A     | 556 | C    |
| 11  | A     | 557 | A    |
| 11  | A     | 558 | A    |
| 11  | A     | 559 | C    |
| 11  | A     | 560 | A    |
| 11  | A     | 561 | U    |
| 11  | A     | 564 | U    |
| 11  | A     | 565 | C    |
| 11  | A     | 566 | C    |
| 11  | A     | 568 | A    |
| 11  | A     | 570 | A    |
| 11  | A     | 571 | A    |
| 11  | A     | 572 | A    |
| 11  | A     | 573 | C    |
| 11  | A     | 574 | U    |
| 11  | A     | 575 | A    |
| 11  | A     | 577 | U    |
| 11  | A     | 578 | A    |
| 11  | A     | 579 | A    |
| 11  | A     | 582 | A    |
| 11  | A     | 583 | A    |
| 11  | A     | 584 | C    |
| 11  | A     | 588 | U    |
| 11  | A     | 590 | G    |
| 11  | A     | 591 | C    |
| 11  | A     | 593 | C    |
| 11  | A     | 594 | A    |
| 11  | A     | 596 | U    |
| 11  | A     | 597 | A    |
| 11  | A     | 601 | G    |
| 11  | A     | 603 | C    |
| 11  | A     | 610 | A    |
| 11  | A     | 611 | U    |
| 11  | A     | 612 | U    |
| 11  | A     | 613 | G    |
| 11  | A     | 614 | A    |
| 11  | A     | 615 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11  | A     | 616 | A    |
| 11  | A     | 617 | C    |
| 11  | A     | 618 | A    |
| 11  | A     | 623 | A    |
| 11  | A     | 627 | A    |
| 11  | A     | 628 | U    |
| 11  | A     | 629 | A    |
| 11  | A     | 631 | U    |
| 11  | A     | 632 | G    |
| 11  | A     | 638 | A    |
| 11  | A     | 641 | A    |
| 11  | A     | 647 | A    |
| 11  | A     | 648 | A    |
| 11  | A     | 650 | A    |
| 11  | A     | 652 | G    |
| 11  | A     | 653 | C    |
| 11  | A     | 654 | C    |
| 11  | A     | 655 | U    |
| 11  | A     | 656 | U    |
| 11  | A     | 659 | U    |
| 11  | A     | 665 | C    |
| 11  | A     | 666 | A    |
| 11  | A     | 672 | U    |
| 11  | A     | 673 | U    |
| 11  | A     | 674 | A    |
| 11  | A     | 682 | A    |
| 11  | A     | 684 | C    |
| 11  | A     | 687 | A    |
| 11  | A     | 688 | U    |
| 11  | A     | 689 | A    |
| 11  | A     | 692 | A    |
| 11  | A     | 693 | U    |
| 11  | A     | 695 | C    |
| 11  | A     | 699 | U    |
| 11  | A     | 700 | A    |
| 11  | A     | 702 | U    |
| 11  | A     | 703 | U    |
| 11  | A     | 705 | A    |
| 11  | A     | 706 | C    |
| 11  | A     | 710 | C    |
| 11  | A     | 711 | A    |
| 11  | A     | 714 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11  | A     | 716 | A    |
| 11  | A     | 717 | C    |
| 11  | A     | 718 | C    |
| 11  | A     | 719 | A    |
| 11  | A     | 720 | A    |
| 11  | A     | 721 | A    |
| 11  | A     | 722 | A    |
| 11  | A     | 723 | C    |
| 11  | A     | 724 | A    |
| 11  | A     | 725 | A    |
| 11  | A     | 726 | C    |
| 11  | A     | 734 | C    |
| 11  | A     | 735 | G    |
| 11  | A     | 737 | U    |
| 11  | A     | 741 | U    |
| 11  | A     | 742 | A    |
| 11  | A     | 743 | A    |
| 11  | A     | 744 | U    |
| 11  | A     | 745 | U    |
| 11  | A     | 746 | A    |
| 11  | A     | 747 | C    |
| 11  | A     | 748 | A    |
| 11  | A     | 751 | G    |
| 11  | A     | 756 | C    |
| 11  | A     | 757 | C    |
| 11  | A     | 761 | C    |
| 11  | A     | 762 | A    |
| 11  | A     | 763 | C    |
| 11  | A     | 764 | A    |
| 11  | A     | 765 | G    |
| 11  | A     | 766 | G    |
| 11  | A     | 772 | A    |
| 11  | A     | 774 | C    |
| 11  | A     | 776 | A    |
| 11  | A     | 777 | G    |
| 11  | A     | 778 | G    |
| 11  | A     | 779 | A    |
| 11  | A     | 780 | A    |
| 11  | A     | 781 | A    |
| 11  | A     | 782 | G    |
| 11  | A     | 783 | A    |
| 11  | A     | 784 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11  | A     | 786 | A    |
| 11  | A     | 787 | A    |
| 11  | A     | 790 | G    |
| 11  | A     | 802 | A    |
| 11  | A     | 803 | C    |
| 11  | A     | 807 | G    |
| 11  | A     | 809 | A    |
| 11  | A     | 811 | A    |
| 11  | A     | 812 | C    |
| 11  | A     | 813 | A    |
| 11  | A     | 815 | A    |
| 11  | A     | 816 | A    |
| 11  | A     | 823 | C    |
| 11  | A     | 825 | U    |
| 11  | A     | 826 | G    |
| 11  | A     | 827 | U    |
| 11  | A     | 828 | U    |
| 11  | A     | 831 | C    |
| 11  | A     | 832 | C    |
| 11  | A     | 833 | A    |
| 11  | A     | 834 | A    |
| 11  | A     | 836 | A    |
| 11  | A     | 842 | A    |
| 11  | A     | 845 | U    |
| 11  | A     | 846 | C    |
| 11  | A     | 847 | U    |
| 11  | A     | 848 | A    |
| 11  | A     | 850 | C    |
| 11  | A     | 851 | A    |
| 11  | A     | 852 | U    |
| 11  | A     | 853 | U    |
| 11  | A     | 854 | A    |
| 11  | A     | 856 | U    |
| 11  | A     | 857 | A    |
| 11  | A     | 858 | G    |
| 11  | A     | 861 | U    |
| 11  | A     | 862 | U    |
| 11  | A     | 866 | G    |
| 11  | A     | 870 | A    |
| 11  | A     | 876 | G    |
| 11  | A     | 879 | C    |
| 11  | A     | 880 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11  | A     | 883 | G    |
| 11  | A     | 884 | A    |
| 11  | A     | 885 | C    |
| 11  | A     | 886 | A    |
| 11  | A     | 890 | G    |
| 11  | A     | 894 | A    |
| 11  | A     | 895 | A    |
| 11  | A     | 897 | G    |
| 11  | A     | 898 | G    |
| 11  | A     | 900 | C    |
| 11  | A     | 901 | G    |
| 11  | A     | 903 | G    |
| 11  | A     | 905 | U    |
| 11  | A     | 906 | A    |
| 11  | A     | 912 | A    |
| 11  | A     | 913 | C    |
| 11  | A     | 914 | C    |
| 11  | A     | 918 | C    |
| 11  | A     | 920 | A    |
| 11  | A     | 921 | A    |
| 11  | A     | 922 | G    |
| 11  | A     | 923 | G    |
| 11  | A     | 924 | U    |
| 11  | A     | 925 | A    |
| 11  | A     | 926 | G    |
| 11  | A     | 929 | U    |
| 11  | A     | 930 | A    |
| 11  | A     | 931 | A    |
| 11  | A     | 932 | U    |
| 11  | A     | 933 | C    |
| 11  | A     | 936 | U    |
| 11  | A     | 937 | U    |
| 11  | A     | 938 | G    |
| 11  | A     | 944 | C    |
| 11  | A     | 947 | A    |
| 11  | A     | 948 | U    |
| 11  | A     | 955 | U    |
| 11  | A     | 956 | U    |
| 11  | A     | 957 | G    |
| 11  | A     | 958 | U    |
| 11  | A     | 959 | A    |
| 11  | A     | 960 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 11  | A     | 962  | A    |
| 11  | A     | 963  | A    |
| 11  | A     | 965  | G    |
| 11  | A     | 968  | C    |
| 11  | A     | 970  | C    |
| 11  | A     | 971  | A    |
| 11  | A     | 972  | C    |
| 11  | A     | 973  | G    |
| 11  | A     | 974  | A    |
| 11  | A     | 975  | G    |
| 11  | A     | 976  | G    |
| 11  | A     | 977  | G    |
| 11  | A     | 978  | U    |
| 11  | A     | 979  | U    |
| 11  | A     | 980  | U    |
| 11  | A     | 984  | U    |
| 11  | A     | 985  | G    |
| 11  | A     | 986  | U    |
| 11  | A     | 989  | C    |
| 11  | A     | 990  | U    |
| 11  | A     | 996  | C    |
| 11  | A     | 997  | C    |
| 11  | A     | 1003 | G    |
| 11  | A     | 1006 | A    |
| 11  | A     | 1014 | C    |
| 11  | A     | 1015 | U    |
| 11  | A     | 1016 | U    |
| 11  | A     | 1023 | A    |
| 11  | A     | 1024 | A    |
| 11  | A     | 1025 | G    |
| 11  | A     | 1026 | A    |
| 11  | A     | 1029 | C    |
| 11  | A     | 1036 | A    |
| 11  | A     | 1038 | A    |
| 11  | A     | 1042 | A    |
| 11  | A     | 1048 | C    |
| 11  | A     | 1049 | G    |
| 11  | A     | 1050 | A    |
| 11  | A     | 1051 | G    |
| 11  | A     | 1052 | A    |
| 11  | A     | 1053 | A    |
| 11  | A     | 1054 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 11  | A     | 1055 | A    |
| 11  | A     | 1056 | C    |
| 11  | A     | 1059 | U    |
| 11  | A     | 1061 | U    |
| 11  | A     | 1062 | G    |
| 11  | A     | 1067 | U    |
| 11  | A     | 1072 | U    |
| 11  | A     | 1073 | U    |
| 11  | A     | 1078 | A    |
| 11  | A     | 1083 | A    |
| 11  | A     | 1086 | A    |
| 11  | A     | 1087 | G    |
| 11  | A     | 1088 | U    |
| 11  | A     | 1089 | U    |
| 11  | A     | 1125 | A    |
| 11  | A     | 1126 | A    |
| 11  | A     | 1134 | U    |
| 11  | A     | 1135 | A    |
| 11  | A     | 1136 | G    |
| 11  | A     | 1139 | A    |
| 11  | A     | 1140 | U    |
| 11  | A     | 1141 | U    |
| 11  | A     | 1144 | G    |
| 11  | A     | 1146 | U    |
| 11  | A     | 1147 | U    |
| 11  | A     | 1148 | G    |
| 11  | A     | 1149 | G    |
| 11  | A     | 1150 | G    |
| 11  | A     | 1157 | U    |
| 11  | A     | 1161 | A    |
| 11  | A     | 1162 | G    |
| 11  | A     | 1163 | U    |
| 11  | A     | 1164 | A    |
| 11  | A     | 1165 | C    |
| 11  | A     | 1166 | A    |
| 11  | A     | 1167 | A    |
| 11  | A     | 1176 | C    |
| 11  | A     | 1178 | G    |
| 11  | A     | 1180 | G    |
| 11  | A     | 1181 | U    |
| 11  | A     | 1184 | U    |
| 11  | A     | 1185 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 11  | A     | 1186 | U    |
| 11  | A     | 1187 | U    |
| 11  | A     | 1189 | A    |
| 11  | A     | 1193 | A    |
| 11  | A     | 1204 | U    |
| 11  | A     | 1205 | C    |
| 11  | A     | 1210 | U    |
| 11  | A     | 1211 | A    |
| 11  | A     | 1224 | C    |
| 11  | A     | 1225 | U    |
| 11  | A     | 1226 | U    |
| 11  | A     | 1227 | A    |
| 11  | A     | 1229 | U    |
| 11  | A     | 1230 | G    |
| 11  | A     | 1232 | U    |
| 11  | A     | 1233 | C    |
| 11  | A     | 1236 | A    |
| 11  | A     | 1237 | A    |
| 11  | A     | 1238 | A    |
| 11  | A     | 1239 | U    |
| 11  | A     | 1240 | U    |
| 11  | A     | 1241 | U    |
| 11  | A     | 1243 | G    |
| 11  | A     | 1244 | A    |
| 11  | A     | 1245 | U    |
| 11  | A     | 1246 | C    |
| 11  | A     | 1247 | A    |
| 11  | A     | 1250 | G    |
| 11  | A     | 1251 | G    |
| 11  | A     | 1252 | A    |
| 11  | A     | 1256 | A    |
| 11  | A     | 1257 | G    |
| 11  | A     | 1258 | U    |
| 11  | A     | 1262 | C    |
| 11  | A     | 1268 | G    |
| 11  | A     | 1269 | A    |
| 11  | A     | 1270 | U    |
| 11  | A     | 1277 | G    |
| 11  | A     | 1285 | G    |
| 11  | A     | 1289 | U    |
| 11  | A     | 1290 | A    |
| 11  | A     | 1292 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 11  | A     | 1294 | U    |
| 11  | A     | 1295 | U    |
| 11  | A     | 1297 | C    |
| 11  | A     | 1301 | C    |
| 11  | A     | 1302 | G    |
| 11  | A     | 1305 | A    |
| 11  | A     | 1308 | A    |
| 11  | A     | 1309 | G    |
| 11  | A     | 1312 | U    |
| 11  | A     | 1313 | U    |
| 11  | A     | 1315 | A    |
| 11  | A     | 1317 | G    |
| 11  | A     | 1323 | G    |
| 11  | A     | 1324 | A    |
| 11  | A     | 1326 | G    |
| 11  | A     | 1327 | U    |
| 11  | A     | 1328 | U    |
| 11  | A     | 1330 | G    |
| 11  | A     | 1334 | A    |
| 11  | A     | 1339 | A    |
| 11  | A     | 1340 | C    |
| 11  | A     | 1341 | C    |
| 11  | A     | 1342 | C    |
| 11  | A     | 1345 | A    |
| 11  | A     | 1346 | U    |
| 11  | A     | 1348 | G    |
| 11  | A     | 1349 | U    |
| 11  | A     | 1350 | G    |
| 11  | A     | 1351 | C    |
| 11  | A     | 1352 | A    |
| 11  | A     | 1355 | C    |
| 11  | A     | 1356 | G    |
| 11  | A     | 1363 | A    |
| 11  | A     | 1364 | A    |
| 11  | A     | 1372 | U    |
| 11  | A     | 1375 | U    |
| 11  | A     | 1376 | U    |
| 11  | A     | 1383 | U    |
| 11  | A     | 1385 | A    |
| 11  | A     | 1387 | A    |
| 11  | A     | 1388 | G    |
| 11  | A     | 1394 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 11  | A     | 1397 | G    |
| 11  | A     | 1400 | C    |
| 11  | A     | 1402 | G    |
| 11  | A     | 1406 | U    |
| 11  | A     | 1407 | C    |
| 11  | A     | 1409 | G    |
| 11  | A     | 1411 | C    |
| 11  | A     | 1412 | C    |
| 11  | A     | 1413 | G    |
| 11  | A     | 1414 | G    |
| 11  | A     | 1416 | G    |
| 11  | A     | 1423 | A    |
| 11  | A     | 1426 | U    |
| 11  | A     | 1427 | C    |
| 11  | A     | 1431 | U    |
| 11  | A     | 1432 | U    |
| 11  | A     | 1434 | U    |
| 11  | A     | 1442 | A    |
| 11  | A     | 1443 | U    |
| 11  | A     | 1446 | A    |
| 11  | A     | 1449 | U    |
| 11  | A     | 1450 | C    |
| 11  | A     | 1453 | C    |
| 11  | A     | 1454 | C    |
| 11  | A     | 1455 | A    |
| 11  | A     | 1456 | G    |
| 11  | A     | 1457 | U    |
| 11  | A     | 1458 | A    |
| 11  | A     | 1463 | A    |
| 11  | A     | 1465 | G    |
| 11  | A     | 1466 | A    |
| 11  | A     | 1468 | A    |
| 11  | A     | 1472 | G    |
| 11  | A     | 1474 | A    |
| 11  | A     | 1478 | G    |
| 11  | A     | 1480 | A    |
| 11  | A     | 1488 | C    |
| 11  | A     | 1490 | C    |
| 11  | A     | 1491 | A    |
| 11  | A     | 1492 | A    |
| 11  | A     | 1496 | C    |
| 11  | A     | 1500 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 11  | A     | 1502 | A    |
| 11  | A     | 1503 | G    |
| 11  | A     | 1507 | U    |
| 11  | A     | 1508 | A    |
| 11  | A     | 1510 | U    |
| 11  | A     | 1511 | U    |
| 11  | A     | 1513 | A    |
| 11  | A     | 1514 | U    |
| 11  | A     | 1516 | A    |
| 11  | A     | 1518 | U    |
| 11  | A     | 1519 | U    |
| 11  | A     | 1520 | A    |
| 11  | A     | 1522 | U    |
| 11  | A     | 1523 | C    |
| 11  | A     | 1524 | U    |
| 11  | A     | 1525 | U    |
| 11  | A     | 1526 | A    |
| 11  | A     | 1529 | C    |
| 11  | A     | 1530 | U    |
| 11  | A     | 1531 | A    |
| 11  | A     | 1534 | U    |
| 11  | A     | 1536 | A    |
| 11  | A     | 1537 | C    |
| 11  | A     | 1541 | U    |
| 11  | A     | 1542 | A    |
| 11  | A     | 1543 | A    |
| 11  | A     | 1544 | U    |
| 11  | A     | 1545 | A    |
| 11  | A     | 1546 | A    |
| 11  | A     | 1547 | A    |
| 11  | A     | 1549 | C    |
| 11  | A     | 1550 | C    |
| 11  | A     | 1551 | A    |
| 11  | A     | 1552 | G    |
| 11  | A     | 1556 | U    |
| 11  | A     | 1557 | A    |
| 11  | A     | 1560 | A    |
| 11  | A     | 1565 | G    |
| 11  | A     | 1566 | C    |
| 11  | A     | 1567 | A    |
| 11  | A     | 1568 | C    |
| 11  | A     | 1569 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13  | C     | 75  | C    |
| 13  | C     | 76  | A    |

All (29) RNA pucker outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 11  | A     | 39   | A    |
| 11  | A     | 48   | U    |
| 11  | A     | 160  | A    |
| 11  | A     | 204  | A    |
| 11  | A     | 335  | A    |
| 11  | A     | 347  | G    |
| 11  | A     | 350  | A    |
| 11  | A     | 374  | U    |
| 11  | A     | 446  | A    |
| 11  | A     | 512  | A    |
| 11  | A     | 521  | U    |
| 11  | A     | 555  | C    |
| 11  | A     | 556  | C    |
| 11  | A     | 569  | A    |
| 11  | A     | 572  | A    |
| 11  | A     | 573  | C    |
| 11  | A     | 583  | A    |
| 11  | A     | 617  | C    |
| 11  | A     | 762  | A    |
| 11  | A     | 875  | U    |
| 11  | A     | 912  | A    |
| 11  | A     | 931  | A    |
| 11  | A     | 936  | U    |
| 11  | A     | 937  | U    |
| 11  | A     | 1139 | A    |
| 11  | A     | 1140 | U    |
| 11  | A     | 1431 | U    |
| 11  | A     | 1467 | C    |
| 11  | A     | 1518 | U    |

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

62 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 12  | P5P  | B     | 1   | 12   | 21,24,24     | 1.37 | 2 (9%)   | 21,36,36    | 1.71 | 3 (14%)  |
| 12  | P5P  | B     | 10  | 12   | 16,23,24     | 1.29 | 3 (18%)  | 15,33,36    | 1.88 | 3 (20%)  |
| 12  | Y5P  | B     | 11  | 12   | 14,19,20     | 4.94 | 3 (21%)  | 18,26,29    | 1.71 | 1 (5%)   |
| 12  | Y5P  | B     | 12  | 12   | 14,19,20     | 3.17 | 2 (14%)  | 18,26,29    | 2.85 | 2 (11%)  |
| 12  | Y5P  | B     | 13  | 12   | 14,19,20     | 3.30 | 2 (14%)  | 18,26,29    | 3.16 | 2 (11%)  |
| 12  | P5P  | B     | 14  | 12   | 16,23,24     | 0.73 | 0        | 15,33,36    | 0.82 | 0        |
| 12  | P5P  | B     | 15  | 12   | 16,23,24     | 0.74 | 0        | 15,33,36    | 0.80 | 1 (6%)   |
| 12  | Y5P  | B     | 2   | 12   | 14,19,20     | 3.21 | 2 (14%)  | 18,26,29    | 2.85 | 2 (11%)  |
| 12  | P5P  | B     | 23  | 12   | 16,23,24     | 0.81 | 0        | 15,33,36    | 0.89 | 0        |
| 12  | P5P  | B     | 24  | 12   | 16,23,24     | 0.76 | 0        | 15,33,36    | 0.79 | 0        |
| 12  | P5P  | B     | 25  | 12   | 16,23,24     | 1.33 | 3 (18%)  | 15,33,36    | 2.13 | 3 (20%)  |
| 12  | Y5P  | B     | 26  | 12   | 14,19,20     | 4.80 | 3 (21%)  | 18,26,29    | 1.88 | 1 (5%)   |
| 12  | P5P  | B     | 27  | 12   | 16,23,24     | 0.72 | 0        | 15,33,36    | 1.08 | 1 (6%)   |
| 12  | P5P  | B     | 28  | 12   | 16,23,24     | 0.78 | 0        | 15,33,36    | 0.71 | 0        |
| 12  | P5P  | B     | 29  | 12   | 16,23,24     | 1.37 | 2 (12%)  | 15,33,36    | 2.13 | 3 (20%)  |
| 12  | Y5P  | B     | 3   | 12   | 14,19,20     | 3.24 | 2 (14%)  | 18,26,29    | 3.16 | 2 (11%)  |
| 12  | P5P  | B     | 30  | 12   | 16,23,24     | 1.33 | 3 (18%)  | 15,33,36    | 1.89 | 3 (20%)  |
| 12  | Y5P  | B     | 31  | 12   | 14,19,20     | 5.02 | 3 (21%)  | 18,26,29    | 1.68 | 1 (5%)   |
| 12  | P5P  | B     | 32  | 12   | 16,23,24     | 0.73 | 0        | 15,33,36    | 0.80 | 0        |
| 12  | Y5P  | B     | 33  | 12   | 14,19,20     | 4.99 | 3 (21%)  | 18,26,29    | 1.68 | 1 (5%)   |
| 12  | Y5P  | B     | 34  | 12   | 14,19,20     | 3.20 | 2 (14%)  | 18,26,29    | 2.83 | 2 (11%)  |
| 12  | P5P  | B     | 35  | 12   | 16,23,24     | 1.50 | 2 (12%)  | 15,33,36    | 1.76 | 2 (13%)  |
| 12  | P5P  | B     | 36  | 12   | 16,23,24     | 0.75 | 0        | 15,33,36    | 0.95 | 0        |
| 12  | P5P  | B     | 37  | 12   | 16,23,24     | 0.74 | 0        | 15,33,36    | 0.81 | 0        |
| 12  | P5P  | B     | 38  | 12   | 16,23,24     | 0.71 | 0        | 15,33,36    | 0.96 | 0        |
| 12  | P5P  | B     | 39  | 12   | 16,23,24     | 0.72 | 0        | 15,33,36    | 0.91 | 1 (6%)   |
| 12  | P5P  | B     | 4   | 12   | 16,23,24     | 0.74 | 0        | 15,33,36    | 0.73 | 0        |
| 12  | Y5P  | B     | 40  | 12   | 14,19,20     | 3.33 | 2 (14%)  | 18,26,29    | 2.86 | 2 (11%)  |
| 12  | P5P  | B     | 41  | 12   | 16,23,24     | 1.31 | 2 (12%)  | 15,33,36    | 1.76 | 2 (13%)  |
| 12  | Y5P  | B     | 42  | 12   | 14,19,20     | 4.84 | 3 (21%)  | 18,26,29    | 1.78 | 1 (5%)   |
| 12  | Y5P  | B     | 43  | 12   | 14,19,20     | 5.06 | 3 (21%)  | 18,26,29    | 1.65 | 1 (5%)   |
| 12  | Y5P  | B     | 44  | 12   | 14,19,20     | 3.14 | 2 (14%)  | 18,26,29    | 2.76 | 2 (11%)  |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 12  | P5P  | B     | 45  | 12   | 16,23,24     | 0.73 | 0        | 15,33,36    | 0.79 | 0        |
| 12  | P5P  | B     | 46  | 12   | 16,23,24     | 1.31 | 3 (18%)  | 15,33,36    | 1.87 | 2 (13%)  |
| 12  | P5P  | B     | 47  | 12   | 16,23,24     | 0.75 | 1 (6%)   | 15,33,36    | 0.87 | 1 (6%)   |
| 12  | Y5P  | B     | 48  | 12   | 14,19,20     | 3.28 | 2 (14%)  | 18,26,29    | 2.82 | 2 (11%)  |
| 12  | P5P  | B     | 49  | 12   | 16,23,24     | 1.43 | 2 (12%)  | 15,33,36    | 1.96 | 2 (13%)  |
| 12  | P5P  | B     | 5   | 12   | 16,23,24     | 0.73 | 0        | 15,33,36    | 0.81 | 1 (6%)   |
| 12  | P5P  | B     | 50  | 12   | 16,23,24     | 0.77 | 0        | 15,33,36    | 0.82 | 0        |
| 12  | P5P  | B     | 51  | 12   | 16,23,24     | 1.40 | 2 (12%)  | 15,33,36    | 1.93 | 2 (13%)  |
| 12  | Y5P  | B     | 52  | 12   | 14,19,20     | 4.82 | 3 (21%)  | 18,26,29    | 1.83 | 1 (5%)   |
| 12  | Y5P  | B     | 53  | 12   | 14,19,20     | 4.87 | 3 (21%)  | 18,26,29    | 1.82 | 1 (5%)   |
| 12  | P5P  | B     | 58  | 12   | 16,23,24     | 0.73 | 0        | 15,33,36    | 0.76 | 0        |
| 12  | P5P  | B     | 59  | 12   | 16,23,24     | 1.41 | 2 (12%)  | 15,33,36    | 1.93 | 2 (13%)  |
| 12  | Y5P  | B     | 6   | 12   | 14,19,20     | 3.22 | 2 (14%)  | 18,26,29    | 2.93 | 2 (11%)  |
| 12  | Y5P  | B     | 60  | 12   | 14,19,20     | 4.75 | 3 (21%)  | 18,26,29    | 1.83 | 1 (5%)   |
| 12  | Y5P  | B     | 61  | 12   | 14,19,20     | 3.21 | 3 (21%)  | 18,26,29    | 2.85 | 2 (11%)  |
| 12  | Y5P  | B     | 62  | 12   | 14,19,20     | 3.21 | 2 (14%)  | 18,26,29    | 2.92 | 2 (11%)  |
| 12  | Y5P  | B     | 63  | 12   | 14,19,20     | 4.87 | 3 (21%)  | 18,26,29    | 1.78 | 1 (5%)   |
| 12  | P5P  | B     | 64  | 12   | 16,23,24     | 0.72 | 0        | 15,33,36    | 0.85 | 0        |
| 12  | Y5P  | B     | 65  | 12   | 14,19,20     | 3.23 | 2 (14%)  | 18,26,29    | 2.94 | 2 (11%)  |
| 12  | P5P  | B     | 66  | 12   | 16,23,24     | 0.77 | 1 (6%)   | 15,33,36    | 0.69 | 0        |
| 12  | P5P  | B     | 67  | 12   | 16,23,24     | 0.75 | 0        | 15,33,36    | 0.86 | 1 (6%)   |
| 12  | P5P  | B     | 68  | 12   | 16,23,24     | 0.74 | 0        | 15,33,36    | 0.80 | 0        |
| 12  | Y5P  | B     | 69  | 12   | 14,19,20     | 4.78 | 3 (21%)  | 18,26,29    | 1.73 | 1 (5%)   |
| 12  | P5P  | B     | 7   | 12   | 16,23,24     | 1.40 | 2 (12%)  | 15,33,36    | 2.00 | 2 (13%)  |
| 12  | P5P  | B     | 70  | 12   | 16,23,24     | 0.73 | 0        | 15,33,36    | 0.73 | 0        |
| 12  | Y5P  | B     | 71  | 12   | 14,19,20     | 4.85 | 3 (21%)  | 18,26,29    | 1.76 | 1 (5%)   |
| 12  | Y5P  | B     | 72  | 12   | 14,19,20     | 4.87 | 3 (21%)  | 18,26,29    | 1.73 | 1 (5%)   |
| 12  | P5P  | B     | 73  | 12   | 16,23,24     | 0.75 | 1 (6%)   | 15,33,36    | 0.63 | 0        |
| 12  | Y5P  | B     | 8   | 12   | 14,19,20     | 3.11 | 2 (14%)  | 18,26,29    | 3.20 | 2 (11%)  |
| 12  | P5P  | B     | 9   | 12   | 16,23,24     | 0.77 | 0        | 15,33,36    | 0.72 | 0        |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 12  | P5P  | B     | 1   | 12   | -       | 0/6/26/26 | 0/3/3/3 |
| 12  | P5P  | B     | 10  | 12   | -       | 0/3/25/26 | 0/3/3/3 |
| 12  | Y5P  | B     | 11  | 12   | -       | 0/7/33/34 | 0/2/2/2 |
| 12  | Y5P  | B     | 12  | 12   | -       | 0/7/33/34 | 0/2/2/2 |
| 12  | Y5P  | B     | 13  | 12   | -       | 0/7/33/34 | 0/2/2/2 |
| 12  | P5P  | B     | 14  | 12   | -       | 0/3/25/26 | 0/3/3/3 |
| 12  | P5P  | B     | 15  | 12   | -       | 0/3/25/26 | 0/3/3/3 |
| 12  | Y5P  | B     | 2   | 12   | -       | 0/7/33/34 | 0/2/2/2 |
| 12  | P5P  | B     | 23  | 12   | -       | 0/3/25/26 | 0/3/3/3 |
| 12  | P5P  | B     | 24  | 12   | -       | 0/3/25/26 | 0/3/3/3 |
| 12  | P5P  | B     | 25  | 12   | -       | 0/3/25/26 | 0/3/3/3 |
| 12  | Y5P  | B     | 26  | 12   | -       | 0/7/33/34 | 0/2/2/2 |
| 12  | P5P  | B     | 27  | 12   | -       | 0/3/25/26 | 0/3/3/3 |
| 12  | P5P  | B     | 28  | 12   | -       | 0/3/25/26 | 0/3/3/3 |
| 12  | P5P  | B     | 29  | 12   | -       | 0/3/25/26 | 0/3/3/3 |
| 12  | Y5P  | B     | 3   | 12   | -       | 0/7/33/34 | 0/2/2/2 |
| 12  | P5P  | B     | 30  | 12   | -       | 0/3/25/26 | 0/3/3/3 |
| 12  | Y5P  | B     | 31  | 12   | -       | 0/7/33/34 | 0/2/2/2 |
| 12  | P5P  | B     | 32  | 12   | -       | 0/3/25/26 | 0/3/3/3 |
| 12  | Y5P  | B     | 33  | 12   | -       | 0/7/33/34 | 0/2/2/2 |
| 12  | Y5P  | B     | 34  | 12   | -       | 0/7/33/34 | 0/2/2/2 |
| 12  | P5P  | B     | 35  | 12   | -       | 0/3/25/26 | 0/3/3/3 |
| 12  | P5P  | B     | 36  | 12   | -       | 0/3/25/26 | 0/3/3/3 |
| 12  | P5P  | B     | 37  | 12   | -       | 0/3/25/26 | 0/3/3/3 |
| 12  | P5P  | B     | 38  | 12   | -       | 0/3/25/26 | 0/3/3/3 |
| 12  | P5P  | B     | 39  | 12   | -       | 0/3/25/26 | 0/3/3/3 |
| 12  | P5P  | B     | 4   | 12   | -       | 0/3/25/26 | 0/3/3/3 |
| 12  | Y5P  | B     | 40  | 12   | -       | 0/7/33/34 | 0/2/2/2 |
| 12  | P5P  | B     | 41  | 12   | -       | 0/3/25/26 | 0/3/3/3 |
| 12  | Y5P  | B     | 42  | 12   | -       | 0/7/33/34 | 0/2/2/2 |
| 12  | Y5P  | B     | 43  | 12   | -       | 0/7/33/34 | 0/2/2/2 |
| 12  | Y5P  | B     | 44  | 12   | -       | 0/7/33/34 | 0/2/2/2 |
| 12  | P5P  | B     | 45  | 12   | -       | 0/3/25/26 | 0/3/3/3 |
| 12  | P5P  | B     | 46  | 12   | -       | 0/3/25/26 | 0/3/3/3 |
| 12  | P5P  | B     | 47  | 12   | -       | 0/3/25/26 | 0/3/3/3 |
| 12  | Y5P  | B     | 48  | 12   | -       | 0/7/33/34 | 0/2/2/2 |
| 12  | P5P  | B     | 49  | 12   | -       | 0/3/25/26 | 0/3/3/3 |
| 12  | P5P  | B     | 5   | 12   | -       | 0/3/25/26 | 0/3/3/3 |
| 12  | P5P  | B     | 50  | 12   | -       | 0/3/25/26 | 0/3/3/3 |
| 12  | P5P  | B     | 51  | 12   | -       | 0/3/25/26 | 0/3/3/3 |
| 12  | Y5P  | B     | 52  | 12   | -       | 0/7/33/34 | 0/2/2/2 |
| 12  | Y5P  | B     | 53  | 12   | -       | 0/7/33/34 | 0/2/2/2 |
| 12  | P5P  | B     | 58  | 12   | -       | 0/3/25/26 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 12  | P5P  | B     | 59  | 12   | -       | 0/3/25/26 | 0/3/3/3 |
| 12  | Y5P  | B     | 6   | 12   | -       | 0/7/33/34 | 0/2/2/2 |
| 12  | Y5P  | B     | 60  | 12   | -       | 0/7/33/34 | 0/2/2/2 |
| 12  | Y5P  | B     | 61  | 12   | -       | 0/7/33/34 | 0/2/2/2 |
| 12  | Y5P  | B     | 62  | 12   | -       | 0/7/33/34 | 0/2/2/2 |
| 12  | Y5P  | B     | 63  | 12   | -       | 0/7/33/34 | 0/2/2/2 |
| 12  | P5P  | B     | 64  | 12   | -       | 0/3/25/26 | 0/3/3/3 |
| 12  | Y5P  | B     | 65  | 12   | -       | 0/7/33/34 | 0/2/2/2 |
| 12  | P5P  | B     | 66  | 12   | -       | 0/3/25/26 | 0/3/3/3 |
| 12  | P5P  | B     | 67  | 12   | -       | 0/3/25/26 | 0/3/3/3 |
| 12  | P5P  | B     | 68  | 12   | -       | 0/3/25/26 | 0/3/3/3 |
| 12  | Y5P  | B     | 69  | 12   | -       | 0/7/33/34 | 0/2/2/2 |
| 12  | P5P  | B     | 7   | 12   | -       | 0/3/25/26 | 0/3/3/3 |
| 12  | P5P  | B     | 70  | 12   | -       | 0/3/25/26 | 0/3/3/3 |
| 12  | Y5P  | B     | 71  | 12   | -       | 0/7/33/34 | 0/2/2/2 |
| 12  | Y5P  | B     | 72  | 12   | -       | 0/7/33/34 | 0/2/2/2 |
| 12  | P5P  | B     | 73  | 12   | -       | 0/3/25/26 | 0/3/3/3 |
| 12  | Y5P  | B     | 8   | 12   | -       | 0/7/33/34 | 0/2/2/2 |
| 12  | P5P  | B     | 9   | 12   | -       | 0/3/25/26 | 0/3/3/3 |

All (97) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 12  | B     | 43  | Y5P  | C4-N3 | -18.44 | 1.33        | 1.46     |
| 12  | B     | 31  | Y5P  | C4-N3 | -18.38 | 1.33        | 1.46     |
| 12  | B     | 33  | Y5P  | C4-N3 | -18.26 | 1.33        | 1.46     |
| 12  | B     | 11  | Y5P  | C4-N3 | -18.00 | 1.33        | 1.46     |
| 12  | B     | 63  | Y5P  | C4-N3 | -17.70 | 1.34        | 1.46     |
| 12  | B     | 42  | Y5P  | C4-N3 | -17.68 | 1.34        | 1.46     |
| 12  | B     | 53  | Y5P  | C4-N3 | -17.67 | 1.34        | 1.46     |
| 12  | B     | 72  | Y5P  | C4-N3 | -17.64 | 1.34        | 1.46     |
| 12  | B     | 71  | Y5P  | C4-N3 | -17.54 | 1.34        | 1.46     |
| 12  | B     | 26  | Y5P  | C4-N3 | -17.50 | 1.34        | 1.46     |
| 12  | B     | 52  | Y5P  | C4-N3 | -17.47 | 1.34        | 1.46     |
| 12  | B     | 69  | Y5P  | C4-N3 | -17.34 | 1.34        | 1.46     |
| 12  | B     | 60  | Y5P  | C4-N3 | -17.17 | 1.34        | 1.46     |
| 12  | B     | 40  | Y5P  | C4-N3 | -11.71 | 1.38        | 1.46     |
| 12  | B     | 13  | Y5P  | C4-N3 | -11.66 | 1.38        | 1.46     |
| 12  | B     | 48  | Y5P  | C4-N3 | -11.30 | 1.38        | 1.46     |
| 12  | B     | 3   | Y5P  | C4-N3 | -11.27 | 1.38        | 1.46     |
| 12  | B     | 65  | Y5P  | C4-N3 | -11.16 | 1.38        | 1.46     |
| 12  | B     | 6   | Y5P  | C4-N3 | -11.12 | 1.38        | 1.46     |

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| Mol | Chain | Res | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 12  | B     | 2   | Y5P  | C4-N3 | -11.06 | 1.38        | 1.46     |
| 12  | B     | 62  | Y5P  | C4-N3 | -11.04 | 1.38        | 1.46     |
| 12  | B     | 34  | Y5P  | C4-N3 | -11.03 | 1.38        | 1.46     |
| 12  | B     | 61  | Y5P  | C4-N3 | -10.98 | 1.38        | 1.46     |
| 12  | B     | 12  | Y5P  | C4-N3 | -10.89 | 1.38        | 1.46     |
| 12  | B     | 44  | Y5P  | C4-N3 | -10.75 | 1.38        | 1.46     |
| 12  | B     | 8   | Y5P  | C4-N3 | -10.62 | 1.39        | 1.46     |
| 12  | B     | 25  | P5P  | C8-N7 | -2.28  | 1.30        | 1.34     |
| 12  | B     | 30  | P5P  | C8-N7 | -2.22  | 1.30        | 1.34     |
| 12  | B     | 46  | P5P  | C8-N7 | -2.11  | 1.30        | 1.34     |
| 12  | B     | 10  | P5P  | C8-N7 | -2.09  | 1.30        | 1.34     |
| 12  | B     | 47  | P5P  | C6-N1 | 2.02   | 1.36        | 1.32     |
| 12  | B     | 61  | Y5P  | C2-N1 | 2.06   | 1.39        | 1.36     |
| 12  | B     | 30  | P5P  | C2-N1 | 2.11   | 1.37        | 1.33     |
| 12  | B     | 66  | P5P  | C6-N1 | 2.13   | 1.36        | 1.32     |
| 12  | B     | 46  | P5P  | C2-N1 | 2.19   | 1.37        | 1.33     |
| 12  | B     | 73  | P5P  | C6-N1 | 2.21   | 1.36        | 1.32     |
| 12  | B     | 10  | P5P  | C2-N1 | 2.25   | 1.37        | 1.33     |
| 12  | B     | 33  | Y5P  | C2-N1 | 2.26   | 1.40        | 1.36     |
| 12  | B     | 25  | P5P  | C2-N1 | 2.29   | 1.37        | 1.33     |
| 12  | B     | 41  | P5P  | C2-N1 | 2.32   | 1.37        | 1.33     |
| 12  | B     | 29  | P5P  | C2-N1 | 2.33   | 1.37        | 1.33     |
| 12  | B     | 42  | Y5P  | C2-N1 | 2.36   | 1.40        | 1.36     |
| 12  | B     | 26  | Y5P  | C2-N1 | 2.41   | 1.40        | 1.36     |
| 12  | B     | 59  | P5P  | C2-N1 | 2.42   | 1.38        | 1.33     |
| 12  | B     | 7   | P5P  | C2-N1 | 2.43   | 1.38        | 1.33     |
| 12  | B     | 51  | P5P  | C2-N1 | 2.51   | 1.38        | 1.33     |
| 12  | B     | 63  | Y5P  | C2-N1 | 2.52   | 1.40        | 1.36     |
| 12  | B     | 31  | Y5P  | C2-N1 | 2.59   | 1.40        | 1.36     |
| 12  | B     | 49  | P5P  | C2-N1 | 2.62   | 1.38        | 1.33     |
| 12  | B     | 1   | P5P  | C2-N1 | 2.63   | 1.38        | 1.33     |
| 12  | B     | 35  | P5P  | C2-N1 | 2.64   | 1.38        | 1.33     |
| 12  | B     | 43  | Y5P  | C2-N1 | 2.65   | 1.40        | 1.36     |
| 12  | B     | 11  | Y5P  | C2-N1 | 2.69   | 1.40        | 1.36     |
| 12  | B     | 69  | Y5P  | C2-N1 | 2.71   | 1.40        | 1.36     |
| 12  | B     | 31  | Y5P  | C2-N3 | 2.73   | 1.35        | 1.29     |
| 12  | B     | 60  | Y5P  | C2-N1 | 2.83   | 1.41        | 1.36     |
| 12  | B     | 52  | Y5P  | C2-N1 | 2.84   | 1.41        | 1.36     |
| 12  | B     | 53  | Y5P  | C2-N1 | 2.89   | 1.41        | 1.36     |
| 12  | B     | 72  | Y5P  | C2-N1 | 2.91   | 1.41        | 1.36     |
| 12  | B     | 71  | Y5P  | C2-N1 | 2.91   | 1.41        | 1.36     |
| 12  | B     | 33  | Y5P  | C2-N3 | 2.93   | 1.35        | 1.29     |

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| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 12  | B     | 42  | Y5P  | C2-N3 | 3.05 | 1.35        | 1.29     |
| 12  | B     | 26  | Y5P  | C2-N3 | 3.07 | 1.35        | 1.29     |
| 12  | B     | 43  | Y5P  | C2-N3 | 3.07 | 1.35        | 1.29     |
| 12  | B     | 11  | Y5P  | C2-N3 | 3.07 | 1.35        | 1.29     |
| 12  | B     | 69  | Y5P  | C2-N3 | 3.21 | 1.36        | 1.29     |
| 12  | B     | 53  | Y5P  | C2-N3 | 3.23 | 1.36        | 1.29     |
| 12  | B     | 52  | Y5P  | C2-N3 | 3.29 | 1.36        | 1.29     |
| 12  | B     | 60  | Y5P  | C2-N3 | 3.30 | 1.36        | 1.29     |
| 12  | B     | 63  | Y5P  | C2-N3 | 3.30 | 1.36        | 1.29     |
| 12  | B     | 72  | Y5P  | C2-N3 | 3.32 | 1.36        | 1.29     |
| 12  | B     | 71  | Y5P  | C2-N3 | 3.34 | 1.36        | 1.29     |
| 12  | B     | 13  | Y5P  | C2-N3 | 3.64 | 1.37        | 1.29     |
| 12  | B     | 40  | Y5P  | C2-N3 | 3.93 | 1.37        | 1.29     |
| 12  | B     | 25  | P5P  | C6-N1 | 3.96 | 1.39        | 1.32     |
| 12  | B     | 3   | Y5P  | C2-N3 | 3.98 | 1.37        | 1.29     |
| 12  | B     | 10  | P5P  | C6-N1 | 4.03 | 1.39        | 1.32     |
| 12  | B     | 30  | P5P  | C6-N1 | 4.06 | 1.39        | 1.32     |
| 12  | B     | 65  | Y5P  | C2-N3 | 4.07 | 1.38        | 1.29     |
| 12  | B     | 46  | P5P  | C6-N1 | 4.08 | 1.39        | 1.32     |
| 12  | B     | 6   | Y5P  | C2-N3 | 4.10 | 1.38        | 1.29     |
| 12  | B     | 34  | Y5P  | C2-N3 | 4.11 | 1.38        | 1.29     |
| 12  | B     | 2   | Y5P  | C2-N3 | 4.13 | 1.38        | 1.29     |
| 12  | B     | 41  | P5P  | C6-N1 | 4.17 | 1.39        | 1.32     |
| 12  | B     | 12  | Y5P  | C2-N3 | 4.17 | 1.38        | 1.29     |
| 12  | B     | 62  | Y5P  | C2-N3 | 4.17 | 1.38        | 1.29     |
| 12  | B     | 61  | Y5P  | C2-N3 | 4.18 | 1.38        | 1.29     |
| 12  | B     | 48  | Y5P  | C2-N3 | 4.19 | 1.38        | 1.29     |
| 12  | B     | 44  | Y5P  | C2-N3 | 4.24 | 1.38        | 1.29     |
| 12  | B     | 8   | Y5P  | C2-N3 | 4.28 | 1.38        | 1.29     |
| 12  | B     | 29  | P5P  | C6-N1 | 4.38 | 1.40        | 1.32     |
| 12  | B     | 51  | P5P  | C6-N1 | 4.41 | 1.40        | 1.32     |
| 12  | B     | 59  | P5P  | C6-N1 | 4.47 | 1.40        | 1.32     |
| 12  | B     | 7   | P5P  | C6-N1 | 4.48 | 1.40        | 1.32     |
| 12  | B     | 49  | P5P  | C6-N1 | 4.52 | 1.40        | 1.32     |
| 12  | B     | 1   | P5P  | C6-N1 | 4.54 | 1.40        | 1.32     |
| 12  | B     | 35  | P5P  | C6-N1 | 4.77 | 1.40        | 1.32     |

All (74) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|--------|-------------|----------|
| 12  | B     | 8   | Y5P  | N1-C2-N3 | -12.59 | 113.87      | 125.85   |
| 12  | B     | 13  | Y5P  | N1-C2-N3 | -12.57 | 113.89      | 125.85   |

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| Mol | Chain | Res | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 12  | B     | 3   | Y5P  | N1-C2-N3  | -12.46 | 114.00      | 125.85   |
| 12  | B     | 6   | Y5P  | N1-C2-N3  | -11.66 | 114.76      | 125.85   |
| 12  | B     | 65  | Y5P  | N1-C2-N3  | -11.60 | 114.82      | 125.85   |
| 12  | B     | 62  | Y5P  | N1-C2-N3  | -11.56 | 114.85      | 125.85   |
| 12  | B     | 2   | Y5P  | N1-C2-N3  | -11.30 | 115.10      | 125.85   |
| 12  | B     | 12  | Y5P  | N1-C2-N3  | -11.29 | 115.11      | 125.85   |
| 12  | B     | 40  | Y5P  | N1-C2-N3  | -11.26 | 115.14      | 125.85   |
| 12  | B     | 61  | Y5P  | N1-C2-N3  | -11.18 | 115.22      | 125.85   |
| 12  | B     | 34  | Y5P  | N1-C2-N3  | -11.10 | 115.30      | 125.85   |
| 12  | B     | 48  | Y5P  | N1-C2-N3  | -11.07 | 115.32      | 125.85   |
| 12  | B     | 44  | Y5P  | N1-C2-N3  | -10.87 | 115.51      | 125.85   |
| 12  | B     | 26  | Y5P  | N1-C2-N3  | -7.68  | 118.54      | 125.85   |
| 12  | B     | 52  | Y5P  | N1-C2-N3  | -7.44  | 118.77      | 125.85   |
| 12  | B     | 53  | Y5P  | N1-C2-N3  | -7.41  | 118.80      | 125.85   |
| 12  | B     | 60  | Y5P  | N1-C2-N3  | -7.31  | 118.90      | 125.85   |
| 12  | B     | 42  | Y5P  | N1-C2-N3  | -7.22  | 118.98      | 125.85   |
| 12  | B     | 63  | Y5P  | N1-C2-N3  | -7.17  | 119.03      | 125.85   |
| 12  | B     | 71  | Y5P  | N1-C2-N3  | -7.12  | 119.08      | 125.85   |
| 12  | B     | 72  | Y5P  | N1-C2-N3  | -6.98  | 119.21      | 125.85   |
| 12  | B     | 11  | Y5P  | N1-C2-N3  | -6.95  | 119.24      | 125.85   |
| 12  | B     | 33  | Y5P  | N1-C2-N3  | -6.84  | 119.34      | 125.85   |
| 12  | B     | 31  | Y5P  | N1-C2-N3  | -6.77  | 119.41      | 125.85   |
| 12  | B     | 69  | Y5P  | N1-C2-N3  | -6.75  | 119.42      | 125.85   |
| 12  | B     | 43  | Y5P  | N1-C2-N3  | -6.74  | 119.44      | 125.85   |
| 12  | B     | 29  | P5P  | N1-C2-N3  | -3.42  | 123.17      | 127.66   |
| 12  | B     | 59  | P5P  | N1-C2-N3  | -3.20  | 123.45      | 127.66   |
| 12  | B     | 7   | P5P  | N1-C2-N3  | -3.17  | 123.50      | 127.66   |
| 12  | B     | 49  | P5P  | N1-C2-N3  | -3.14  | 123.54      | 127.66   |
| 12  | B     | 51  | P5P  | N1-C2-N3  | -3.08  | 123.61      | 127.66   |
| 12  | B     | 1   | P5P  | N1-C2-N3  | -3.06  | 123.63      | 127.66   |
| 12  | B     | 29  | P5P  | C1'-N9-C4 | -3.01  | 123.45      | 126.81   |
| 12  | B     | 30  | P5P  | N1-C2-N3  | -2.95  | 123.78      | 127.66   |
| 12  | B     | 35  | P5P  | N1-C2-N3  | -2.92  | 123.82      | 127.66   |
| 12  | B     | 46  | P5P  | N1-C2-N3  | -2.87  | 123.89      | 127.66   |
| 12  | B     | 25  | P5P  | N1-C2-N3  | -2.69  | 124.13      | 127.66   |
| 12  | B     | 10  | P5P  | N1-C2-N3  | -2.61  | 124.23      | 127.66   |
| 12  | B     | 41  | P5P  | N1-C2-N3  | -2.46  | 124.42      | 127.66   |
| 12  | B     | 47  | P5P  | C6-N1-C2  | 2.04   | 118.94      | 115.99   |
| 12  | B     | 67  | P5P  | C6-N1-C2  | 2.10   | 119.01      | 115.99   |
| 12  | B     | 10  | P5P  | C1'-N9-C4 | 2.12   | 129.17      | 126.81   |
| 12  | B     | 39  | P5P  | C6-N1-C2  | 2.13   | 119.07      | 115.99   |
| 12  | B     | 15  | P5P  | C6-N1-C2  | 2.15   | 119.08      | 115.99   |

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| Mol | Chain | Res | Type | Atoms     | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|------|-------------|----------|
| 12  | B     | 5   | P5P  | C6-N1-C2  | 2.17 | 119.11      | 115.99   |
| 12  | B     | 30  | P5P  | C1'-N9-C4 | 2.28 | 129.35      | 126.81   |
| 12  | B     | 1   | P5P  | OP2-P-OP1 | 2.39 | 118.42      | 110.63   |
| 12  | B     | 27  | P5P  | C1'-N9-C4 | 3.02 | 130.17      | 126.81   |
| 12  | B     | 40  | Y5P  | C4-N3-C2  | 3.76 | 126.69      | 117.71   |
| 12  | B     | 61  | Y5P  | C4-N3-C2  | 3.79 | 126.76      | 117.71   |
| 12  | B     | 34  | Y5P  | C4-N3-C2  | 3.84 | 126.89      | 117.71   |
| 12  | B     | 44  | Y5P  | C4-N3-C2  | 3.85 | 126.91      | 117.71   |
| 12  | B     | 12  | Y5P  | C4-N3-C2  | 3.85 | 126.91      | 117.71   |
| 12  | B     | 13  | Y5P  | C4-N3-C2  | 3.94 | 127.13      | 117.71   |
| 12  | B     | 6   | Y5P  | C4-N3-C2  | 4.03 | 127.33      | 117.71   |
| 12  | B     | 2   | Y5P  | C4-N3-C2  | 4.03 | 127.34      | 117.71   |
| 12  | B     | 65  | Y5P  | C4-N3-C2  | 4.06 | 127.41      | 117.71   |
| 12  | B     | 25  | P5P  | C1'-N9-C4 | 4.06 | 131.34      | 126.81   |
| 12  | B     | 62  | Y5P  | C4-N3-C2  | 4.10 | 127.51      | 117.71   |
| 12  | B     | 48  | Y5P  | C4-N3-C2  | 4.16 | 127.64      | 117.71   |
| 12  | B     | 8   | Y5P  | C4-N3-C2  | 4.31 | 128.01      | 117.71   |
| 12  | B     | 3   | Y5P  | C4-N3-C2  | 4.57 | 128.64      | 117.71   |
| 12  | B     | 35  | P5P  | C6-N1-C2  | 5.90 | 124.49      | 115.99   |
| 12  | B     | 30  | P5P  | C6-N1-C2  | 6.03 | 124.68      | 115.99   |
| 12  | B     | 41  | P5P  | C6-N1-C2  | 6.06 | 124.72      | 115.99   |
| 12  | B     | 25  | P5P  | C6-N1-C2  | 6.18 | 124.91      | 115.99   |
| 12  | B     | 10  | P5P  | C6-N1-C2  | 6.24 | 124.99      | 115.99   |
| 12  | B     | 46  | P5P  | C6-N1-C2  | 6.37 | 125.17      | 115.99   |
| 12  | B     | 1   | P5P  | C6-N1-C2  | 6.43 | 125.27      | 115.99   |
| 12  | B     | 59  | P5P  | C6-N1-C2  | 6.45 | 125.29      | 115.99   |
| 12  | B     | 51  | P5P  | C6-N1-C2  | 6.45 | 125.29      | 115.99   |
| 12  | B     | 49  | P5P  | C6-N1-C2  | 6.50 | 125.36      | 115.99   |
| 12  | B     | 29  | P5P  | C6-N1-C2  | 6.60 | 125.51      | 115.99   |
| 12  | B     | 7   | P5P  | C6-N1-C2  | 6.72 | 125.68      | 115.99   |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

36 monomers are involved in 29 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 12  | B     | 11  | Y5P  | 1       | 0            |
| 12  | B     | 12  | Y5P  | 1       | 0            |
| 12  | B     | 13  | Y5P  | 1       | 0            |
| 12  | B     | 14  | P5P  | 1       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 12  | B     | 15  | P5P  | 1       | 0            |
| 12  | B     | 23  | P5P  | 3       | 0            |
| 12  | B     | 24  | P5P  | 1       | 0            |
| 12  | B     | 25  | P5P  | 3       | 0            |
| 12  | B     | 26  | Y5P  | 1       | 0            |
| 12  | B     | 3   | Y5P  | 1       | 0            |
| 12  | B     | 30  | P5P  | 1       | 0            |
| 12  | B     | 31  | Y5P  | 1       | 0            |
| 12  | B     | 33  | Y5P  | 1       | 0            |
| 12  | B     | 38  | P5P  | 2       | 0            |
| 12  | B     | 39  | P5P  | 2       | 0            |
| 12  | B     | 4   | P5P  | 2       | 0            |
| 12  | B     | 41  | P5P  | 1       | 0            |
| 12  | B     | 42  | Y5P  | 2       | 0            |
| 12  | B     | 43  | Y5P  | 1       | 0            |
| 12  | B     | 44  | Y5P  | 1       | 0            |
| 12  | B     | 47  | P5P  | 2       | 0            |
| 12  | B     | 48  | Y5P  | 1       | 0            |
| 12  | B     | 49  | P5P  | 1       | 0            |
| 12  | B     | 5   | P5P  | 1       | 0            |
| 12  | B     | 59  | P5P  | 1       | 0            |
| 12  | B     | 60  | Y5P  | 2       | 0            |
| 12  | B     | 61  | Y5P  | 2       | 0            |
| 12  | B     | 62  | Y5P  | 2       | 0            |
| 12  | B     | 63  | Y5P  | 2       | 0            |
| 12  | B     | 67  | P5P  | 1       | 0            |
| 12  | B     | 68  | P5P  | 1       | 0            |
| 12  | B     | 69  | Y5P  | 2       | 0            |
| 12  | B     | 70  | P5P  | 1       | 0            |
| 12  | B     | 71  | Y5P  | 1       | 0            |
| 12  | B     | 72  | Y5P  | 1       | 0            |
| 12  | B     | 9   | P5P  | 2       | 0            |

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 171 ligands modelled in this entry, 171 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.