



## Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 05:34 PM UTC

PDB ID : 9G30 / pdb\_00009g30  
EMDB ID : EMD-50990  
Title : The structure of the Candida albicans ribosome with tRNA-fMet, mRNA, and compounds (GEN and MFQ) shows strong density for the A site tRNA  
Authors : Kolosova, O.; Zgadzay, Y.; Jenner, L.B.; Guskov, A.; Yusupov, M.  
Deposited on : 2024-07-11  
Resolution : 2.35 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

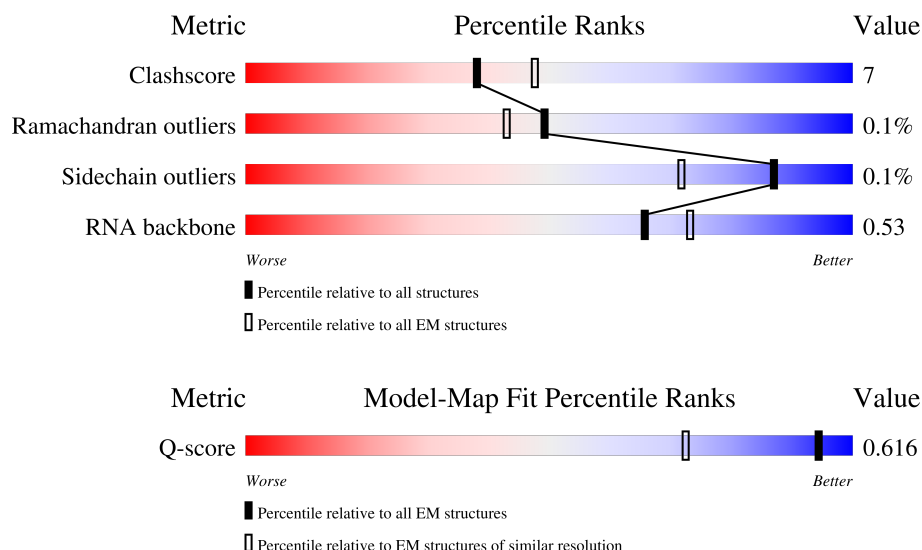
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 1 Overall quality at a glance

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

The reported resolution of this entry is 2.35 Å.

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



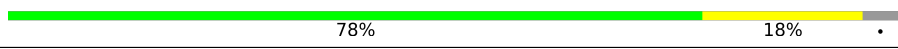
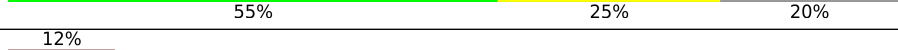
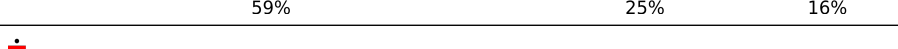
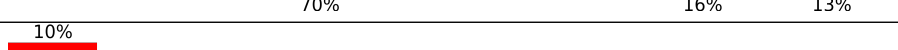
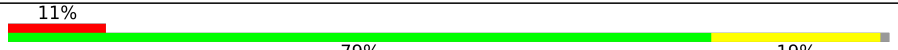
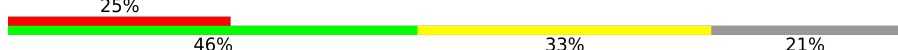
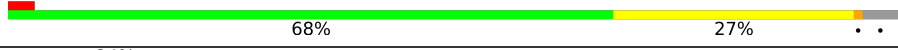
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| RNA backbone          | 8273                        | 3508                        | -                                                        |
| Q-score               | -                           | 25397                       | 4607 ( 1.85 - 2.85 )                                     |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | 0     | 172    |                  |
| 2   | 1     | 3359   |                  |
| 3   | 2     | 160    |                  |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 4   | 3     | 121    |    |
| 5   | 4     | 158    |    |
| 6   | 6     | 137    |    |
| 7   | 7     | 155    |    |
| 8   | 8     | 142    |    |
| 9   | 9     | 127    |    |
| 10  | A     | 1787   |    |
| 11  | B     | 261    |    |
| 12  | C     | 256    |    |
| 13  | D     | 249    |    |
| 14  | E     | 251    |    |
| 15  | F     | 262    |  |
| 16  | G     | 225    |  |
| 17  | H     | 236    |  |
| 18  | I     | 186    |  |
| 19  | J     | 206    |  |
| 20  | K     | 189    |  |
| 21  | L     | 118    |  |
| 22  | M     | 155    |  |
| 23  | N     | 143    |  |
| 24  | O     | 151    |  |
| 25  | P     | 132    |  |
| 26  | Q     | 142    |  |
| 27  | T     | 145    |  |
| 28  | R     | 142    |  |

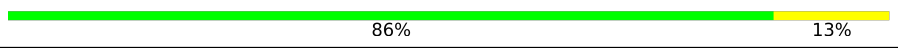
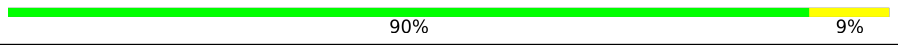
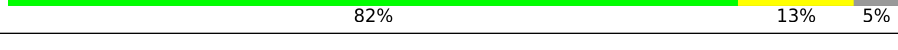
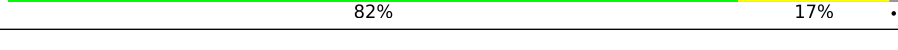
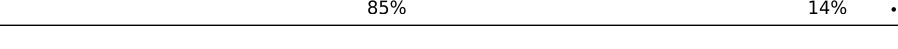
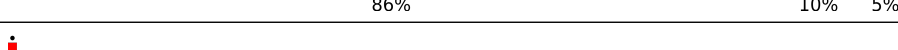
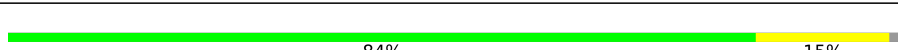
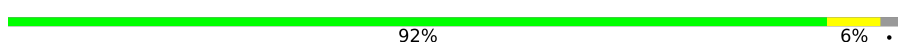
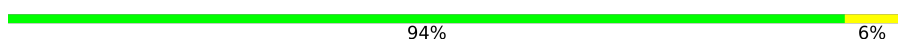
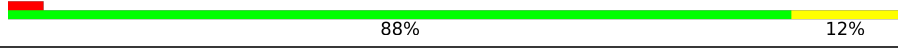
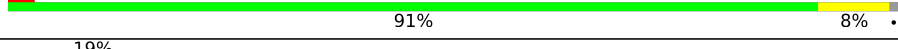
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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 29  | S     | 137    |                  |
| 30  | U     | 145    |                  |
| 31  | V     | 119    |                  |
| 32  | W     | 87     |                  |
| 33  | X     | 130    |                  |
| 34  | Y     | 145    |                  |
| 35  | Z     | 135    |                  |
| 36  | a     | 105    |                  |
| 37  | b     | 119    |                  |
| 38  | c     | 82     |                  |
| 39  | d     | 67     |                  |
| 40  | e     | 56     |                  |
| 41  | f     | 63     |                  |
| 42  | g     | 193    |                  |
| 43  | h     | 317    |                  |
| 44  | j     | 254    |                  |
| 45  | k     | 389    |                  |
| 46  | l     | 363    |                  |
| 47  | m     | 298    |                  |
| 48  | n     | 176    |                  |
| 49  | o     | 241    |                  |
| 50  | p     | 262    |                  |
| 51  | q     | 191    |                  |
| 52  | r     | 220    |                  |
| 53  | s     | 174    |                  |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 54  | t     | 202    |    |
| 55  | u     | 131    |    |
| 56  | v     | 204    |    |
| 57  | w     | 200    |    |
| 58  | x     | 185    |    |
| 59  | y     | 186    |    |
| 60  | z     | 190    |    |
| 61  | AA    | 136    |    |
| 62  | AB    | 149    |    |
| 63  | AC    | 63     |    |
| 64  | AD    | 106    |    |
| 65  | AE    | 112    |  |
| 66  | AF    | 131    |  |
| 67  | AG    | 107    |  |
| 68  | AH    | 122    |  |
| 69  | AI    | 120    |  |
| 70  | AJ    | 99     |  |
| 71  | AK    | 90     |  |
| 72  | AL    | 78     |  |
| 73  | AM    | 51     |  |
| 74  | AN    | 52     |  |
| 75  | AO    | 25     |  |
| 76  | AP    | 106    |  |
| 77  | AQ    | 92     |  |
| 78  | AT    | 77     |  |

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| Mol | Chain | Length | Quality of chain                                                                         |
|-----|-------|--------|------------------------------------------------------------------------------------------|
| 78  | PT    | 77     | <div><div></div><div>23%</div><div>56%</div><div>35%</div><div>8%</div><div></div></div> |
| 79  | MR    | 39     | <div><div></div><div>18%</div><div>10%</div><div>72%</div><div></div></div>              |

## 2 Entry composition

There are 82 unique types of molecules in this entry. The entry contains 197420 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 60S ribosomal protein L20.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 1   | 0     | 171      | Total | C   | N   | O   | S | 2       | 0     |
|     |       |          | 1442  | 933 | 262 | 244 | 3 |         |       |

- Molecule 2 is a RNA chain called 25S rRNA.

| Mol | Chain | Residues | Atoms |       |       |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|-------|
| 2   | 1     | 3066     | Total | C     | N     | O     | P    | 0       | 0     |
|     |       |          | 65536 | 29280 | 11774 | 21416 | 3066 |         |       |

- Molecule 3 is a protein called 60S ribosomal protein L21-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 3   | 2     | 159      | Total | C   | N   | O   | S | 2       | 0     |
|     |       |          | 1276  | 807 | 244 | 223 | 2 |         |       |

- Molecule 4 is a RNA chain called 5S rRNA.

| Mol | Chain | Residues | Atoms |      |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
| 4   | 3     | 121      | Total | C    | N   | O   | P   | 0       | 0     |
|     |       |          | 2579  | 1153 | 463 | 842 | 121 |         |       |

- Molecule 5 is a RNA chain called 5.8S rRNA.

| Mol | Chain | Residues | Atoms |      |     |      |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|-----|---------|-------|
| 5   | 4     | 156      | Total | C    | N   | O    | P   | 0       | 0     |
|     |       |          | 3313  | 1482 | 581 | 1094 | 156 |         |       |

- Molecule 6 is a protein called 60S ribosomal protein L23-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 6   | 6     | 131      | Total | C   | N   | O   | S | 1       | 0     |
|     |       |          | 986   | 621 | 186 | 171 | 8 |         |       |

- Molecule 7 is a protein called 60S ribosomal protein L24-A.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 7   | 7     | 62       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 516   | 328 | 102 | 85 | 1 |         |       |

- Molecule 8 is a protein called 60S ribosomal protein L25.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 8   | 8     | 119      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 960   | 613 | 172 | 174 | 1 |         |       |

- Molecule 9 is a protein called Ribosomal protein L24.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 9   | 9     | 125      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 980   | 613 | 189 | 178 |         |       |

- Molecule 10 is a RNA chain called 18S rRNA.

| Mol | Chain | Residues | Atoms |       |      |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|-------|
| 10  | A     | 1692     | Total | C     | N    | O     | P    | 0       | 0     |
|     |       |          | 36083 | 16130 | 6412 | 11849 | 1692 |         |       |

- Molecule 11 is a protein called 40S ribosomal protein S0.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 11  | B     | 208      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1627  | 1041 | 284 | 297 | 5 |         |       |

- Molecule 12 is a protein called 40S ribosomal protein S1.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 12  | C     | 214      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1724  | 1094 | 313 | 313 | 4 |         |       |

- Molecule 13 is a protein called Ribosomal protein S5.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 13  | D     | 216      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1620  | 1033 | 287 | 295 | 5 |         |       |

- Molecule 14 is a protein called Ribosomal protein S3.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 14  | E     | 222      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1701  | 1084 | 310 | 303 | 4 |         |       |

- Molecule 15 is a protein called 40S ribosomal protein S4.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 15  | F     | 260      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2055  | 1306 | 386 | 358 | 5 |         |       |

- Molecule 16 is a protein called Ribosomal protein S7.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 16  | G     | 199      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1572  | 983 | 294 | 291 | 4 |         |       |

- Molecule 17 is a protein called 40S ribosomal protein S6.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 17  | H     | 226      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1820  | 1133 | 351 | 330 | 6 |         |       |

- Molecule 18 is a protein called 40S ribosomal protein S7.

| Mol | Chain | Residues | Atoms |     |     |     |  | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 18  | I     | 182      | Total | C   | N   | O   |  | 0       | 0     |
|     |       |          | 1466  | 939 | 264 | 263 |  |         |       |

- Molecule 19 is a protein called 40S ribosomal protein S8.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19  | J     | 203      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1579  | 973 | 322 | 283 | 1 |         |       |

- Molecule 20 is a protein called Ribosomal protein S4.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 20  | K     | 178      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1453  | 918 | 286 | 248 | 1 |         |       |

- Molecule 21 is a protein called 40S ribosomal protein S10-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 21  | L     | 93       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 783   | 511 | 129 | 142 | 1 |         |       |

- Molecule 22 is a protein called 40S ribosomal protein S11A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 22  | M     | 141      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1129  | 722 | 212 | 192 | 3 |         |       |

- Molecule 23 is a protein called 40S ribosomal protein S12.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 23  | N     | 71       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 539   | 341 | 95 | 99 | 4 |         |       |

- Molecule 24 is a protein called 40S ribosomal protein S13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 24  | O     | 150      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1187  | 757 | 219 | 210 | 1 |         |       |

- Molecule 25 is a protein called 40S ribosomal protein S14-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 25  | P     | 127      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 942   | 579 | 186 | 174 | 3 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference      |
|-------|---------|----------|--------|----------|----------------|
| P     | 119     | IAS      | ASP    | conflict | UNP A0A8H6F0V4 |

- Molecule 26 is a protein called 40S ribosomal protein S15.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 26  | Q     | 115      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 906   | 578 | 164 | 158 | 6 |         |       |

- Molecule 27 is a protein called 40S ribosomal protein S18-B.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 27  | T     | 142      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1169  | 733 | 228 | 205 | 3 |         |       |

- Molecule 28 is a protein called 40S ribosomal protein S16.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 28  | R     | 141      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1102  | 706 | 202 | 193 | 1 |         |       |

- Molecule 29 is a protein called 40S ribosomal protein S17-B.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 29  | S     | 118      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 954   | 602 | 176 | 175 | 1 |         |       |

- Molecule 30 is a protein called 40S ribosomal protein S19-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 30  | U     | 141      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1100  | 689 | 210 | 200 | 1 |         |       |

- Molecule 31 is a protein called Ribosomal protein S10.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 31  | V     | 100      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 790   | 499 | 146 | 143 | 2 |         |       |

- Molecule 32 is a protein called 40S ribosomal protein S21.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 32  | W     | 87       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 676   | 415 | 126 | 133 | 2 |         |       |

- Molecule 33 is a protein called 40S ribosomal protein S22-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 33  | X     | 129      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1032  | 655 | 191 | 183 | 3 |         |       |

- Molecule 34 is a protein called Ribosomal protein S23 (S12).

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 34  | Y     | 143      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1110  | 701 | 219 | 188 | 2 |         |       |

- Molecule 35 is a protein called 40S ribosomal protein S24.

| Mol | Chain | Residues | Atoms |     |     |     |  | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 35  | Z     | 132      | Total | C   | N   | O   |  | 0       | 0     |
|     |       |          | 1072  | 670 | 216 | 186 |  |         |       |

- Molecule 36 is a protein called 40S ribosomal protein S25.

| Mol | Chain | Residues | Atoms |     |     |     |  | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 36  | a     | 72       | Total | C   | N   | O   |  | 0       | 0     |
|     |       |          | 578   | 369 | 103 | 106 |  |         |       |

- Molecule 37 is a protein called 40S ribosomal protein S26.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 37  | b     | 98       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 779   | 482 | 163 | 128 | 6 |         |       |

- Molecule 38 is a protein called 40S ribosomal protein S27.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 38  | c     | 81       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 614   | 383 | 110 | 114 | 7 |         |       |

- Molecule 39 is a protein called 40S ribosomal protein S28-B.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 39  | d     | 62       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 487   | 299 | 98 | 88 | 2 |         |       |

- Molecule 40 is a protein called 40S ribosomal protein S29A.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 40  | e     | 55       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 454   | 281 | 94 | 75 | 4 |         |       |

- Molecule 41 is a protein called 40S ribosomal protein S30.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 41  | f     | 58       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 461   | 289 | 93 | 77 | 2 |         |       |

- Molecule 42 is a protein called Ubiquitin-40S ribosomal protein S31 fusion protein.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 42  | g     | 70       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 565   | 358 | 111 | 90 | 6 |         |       |

- Molecule 43 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 43  | h     | 241      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1854  | 1176 | 319 | 355 | 4 |         |       |

- Molecule 44 is a protein called 60S ribosomal protein L2-B.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 44  | j     | 249      | Total | C    | N   | O   | S | 1       | 0     |
|     |       |          | 1894  | 1185 | 377 | 330 | 2 |         |       |

- Molecule 45 is a protein called 60S ribosomal protein L3.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 45  | k     | 386      | Total | C    | N   | O   | S | 1       | 0     |
|     |       |          | 3084  | 1955 | 584 | 538 | 7 |         |       |

- Molecule 46 is a protein called 60S ribosomal protein L4-B.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 46  | l     | 361      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2751  | 1729 | 529 | 490 | 3 |         |       |

- Molecule 47 is a protein called 60S ribosomal protein L5.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 47  | m     | 292      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2394  | 1526 | 416 | 450 | 2 |         |       |

- Molecule 48 is a protein called 60S ribosomal protein L6.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 48  | n     | 155      | Total | C   | N   | O   |         |       |
|     |       |          | 1237  | 794 | 226 | 217 | 1       | 0     |

- Molecule 49 is a protein called 60S ribosomal protein L7-A.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 49  | o     | 230      | Total | C    | N   | O   | S |         |       |
|     |       |          | 1860  | 1193 | 343 | 323 | 1 | 1       | 0     |

- Molecule 50 is a protein called 60S ribosomal protein L8.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 50  | p     | 231      | Total | C    | N   | O   | S |         |       |
|     |       |          | 1795  | 1150 | 319 | 323 | 3 | 0       | 0     |

- Molecule 51 is a protein called 60S ribosomal protein L9-B.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 51  | q     | 189      | Total | C   | N   | O   | S |         |       |
|     |       |          | 1510  | 953 | 275 | 278 | 4 | 0       | 0     |

- Molecule 52 is a protein called 60S ribosomal protein L10.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 52  | r     | 218      | Total | C    | N   | O   | S |         |       |
|     |       |          | 1759  | 1110 | 336 | 305 | 8 | 0       | 0     |

- Molecule 53 is a protein called 60S ribosomal protein L11-B.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 53  | s     | 172      | Total | C   | N   | O   | S |         |       |
|     |       |          | 1385  | 864 | 262 | 255 | 4 | 1       | 0     |

- Molecule 54 is a protein called 60S ribosomal protein L13.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 54  | t     | 195      | Total | C   | N   | O   |         |       |
|     |       |          | 1573  | 986 | 311 | 276 | 0       | 0     |

- Molecule 55 is a protein called 60S ribosomal protein L14-B.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 55  | u     | 130      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1029  | 660 | 193 | 175 | 1 |         |       |

- Molecule 56 is a protein called 60S ribosomal protein L15-A.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 56  | v     | 203      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1713  | 1075 | 356 | 280 | 2 |         |       |

- Molecule 57 is a protein called Ribosomal protein L13.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 57  | w     | 199      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1590  | 1025 | 294 | 269 | 2 |         |       |

- Molecule 58 is a protein called Ribosomal protein L22.

| Mol | Chain | Residues | Atoms |     |     |     |  | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 58  | x     | 172      | Total | C   | N   | O   |  | 0       | 0     |
|     |       |          | 1375  | 850 | 279 | 246 |  |         |       |

- Molecule 59 is a protein called 60S ribosomal protein L18-A.

| Mol | Chain | Residues | Atoms |     |     |     |  | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 59  | y     | 185      | Total | C   | N   | O   |  | 3       | 0     |
|     |       |          | 1478  | 930 | 302 | 246 |  |         |       |

- Molecule 60 is a protein called 60S ribosomal protein L19-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 60  | z     | 180      | Total | C   | N   | O   | S | 1       | 0     |
|     |       |          | 1471  | 910 | 313 | 245 | 3 |         |       |

- Molecule 61 is a protein called 60S ribosomal protein L27.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 61  | AA    | 135      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1087  | 705 | 197 | 183 | 2 |         |       |

- Molecule 62 is a protein called 60S ribosomal protein L28.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 62  | AB    | 148      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1170  | 741 | 231 | 197 | 1 |         |       |

- Molecule 63 is a protein called 60S ribosomal protein L29.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 63  | AC    | 60       | Total | C   | N   | O  | S | 1       | 0     |
|     |       |          | 489   | 305 | 105 | 78 | 1 |         |       |

- Molecule 64 is a protein called 60S ribosomal protein L30.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 64  | AD    | 96       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 729   | 469 | 121 | 137 | 2 |         |       |

- Molecule 65 is a protein called 60S ribosomal protein L31-B.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 65  | AE    | 108      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 881   | 558 | 166 | 155 | 2 |         |       |

- Molecule 66 is a protein called 60S ribosomal protein L32.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 66  | AF    | 125      | Total | C   | N   | O   | S | 1       | 0     |
|     |       |          | 1015  | 649 | 197 | 168 | 1 |         |       |

- Molecule 67 is a protein called 60S ribosomal protein L33-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 67  | AG    | 106      | Total | C   | N   | O   | S | 3       | 0     |
|     |       |          | 867   | 558 | 166 | 142 | 1 |         |       |

- Molecule 68 is a protein called 60S ribosomal protein L34-B.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 68  | AH    | 112      | Total | C   | N   | O   | S | 4       | 0     |
|     |       |          | 913   | 567 | 188 | 154 | 4 |         |       |

- Molecule 69 is a protein called Ribosomal protein L29.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 69  | AI    | 119      | Total | C   | N   | O   | 1       | 0     |
|     |       |          | 990   | 629 | 195 | 166 |         |       |

- Molecule 70 is a protein called 60S ribosomal protein L36.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 70  | AJ    | 97       | Total | C   | N   | O   | S | 1       | 0     |
|     |       |          | 764   | 476 | 157 | 130 | 1 |         |       |

- Molecule 71 is a protein called 60S ribosomal protein L37-B.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 71  | AK    | 86       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 677   | 413 | 148 | 110 | 6 |         |       |

- Molecule 72 is a protein called 60S ribosomal protein L38.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 72  | AL    | 77       | Total | C   | N   | O   | 1       | 0     |
|     |       |          | 623   | 398 | 116 | 109 |         |       |

- Molecule 73 is a protein called 60S ribosomal protein L39.

| Mol | Chain | Residues | Atoms |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---------|-------|
| 73  | AM    | 50       | Total | C   | N   | O  | 1       | 0     |
|     |       |          | 446   | 280 | 100 | 66 |         |       |

- Molecule 74 is a protein called 60S ribosomal protein L40-B.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 74  | AN    | 52       | Total | C   | N  | O  | S | 1       | 0     |
|     |       |          | 427   | 265 | 89 | 67 | 6 |         |       |

- Molecule 75 is a protein called 60S ribosomal protein L41.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 75  | AO    | 25       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 236   | 144 | 63 | 28 | 1 |         |       |

- Molecule 76 is a protein called 60S ribosomal protein L42-B.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 76  | AP    | 105      | Total | C   | N   | O   | S | 2       | 0     |
|     |       |          | 863   | 547 | 171 | 140 | 5 |         |       |

- Molecule 77 is a protein called 60S ribosomal protein L43-A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 77  | AQ    | 91       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 698   | 430 | 140 | 124 | 4 |         |       |

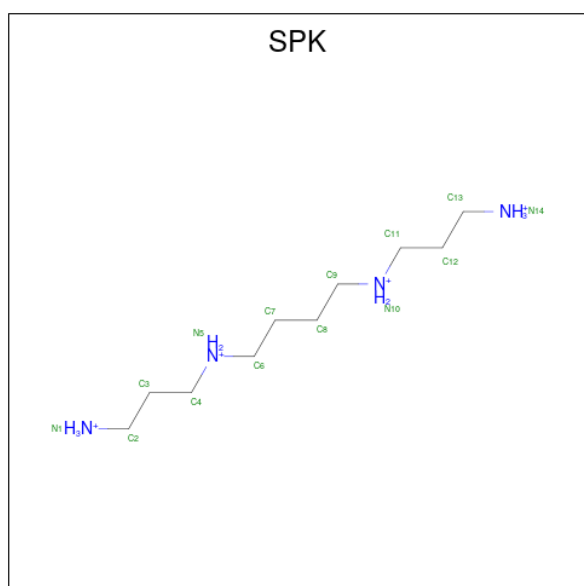
- Molecule 78 is a RNA chain called tRNA.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 78  | PT    | 76       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1623  | 723 | 294 | 530 | 76 |         |       |
| 78  | AT    | 76       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1623  | 723 | 294 | 530 | 76 |         |       |

- Molecule 79 is a RNA chain called mRNA.

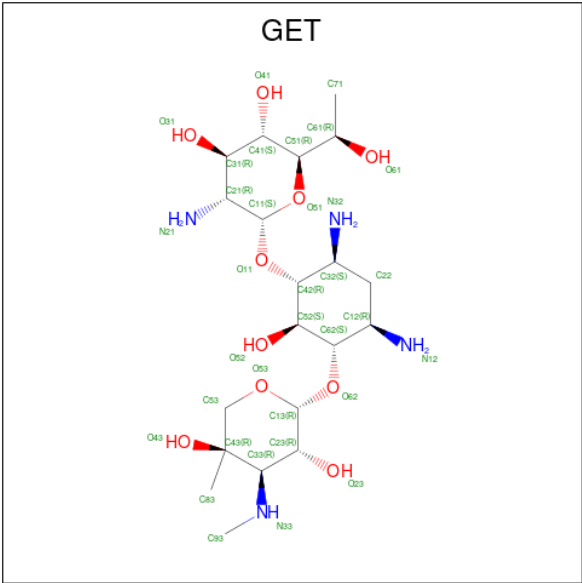
| Mol | Chain | Residues | Atoms |     |    |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|----|---------|-------|
| 79  | MR    | 11       | Total | C   | N  | O  | P  | 0       | 0     |
|     |       |          | 231   | 104 | 39 | 77 | 11 |         |       |

- Molecule 80 is SPERMINE (FULLY PROTONATED FORM) (CCD ID: SPK) (formula:  $C_{10}H_{30}N_4$ ).



| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 80  | 1     | 1        | Total | C  | N | 0       |
|     |       |          | 14    | 10 | 4 |         |

- Molecule 81 is GENETICIN (CCD ID: GET) (formula: C<sub>20</sub>H<sub>40</sub>N<sub>4</sub>O<sub>10</sub>) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |   |    | AltConf |
|-----|-------|----------|-------|----|---|----|---------|
| 81  | 1     | 1        | Total | C  | N | O  | 0       |
|     |       |          | 34    | 20 | 4 | 10 |         |
| 81  | 1     | 1        | Total | C  | N | O  | 0       |
|     |       |          | 34    | 20 | 4 | 10 |         |
| 81  | 1     | 1        | Total | C  | N | O  | 0       |
|     |       |          | 34    | 20 | 4 | 10 |         |
| 81  | 1     | 1        | Total | C  | N | O  | 0       |
|     |       |          | 34    | 20 | 4 | 10 |         |
| 81  | 1     | 1        | Total | C  | N | O  | 0       |
|     |       |          | 34    | 20 | 4 | 10 |         |
| 81  | 1     | 1        | Total | C  | N | O  | 0       |
|     |       |          | 34    | 20 | 4 | 10 |         |
| 81  | 1     | 1        | Total | C  | N | O  | 0       |
|     |       |          | 34    | 20 | 4 | 10 |         |
| 81  | 1     | 1        | Total | C  | N | O  | 0       |
|     |       |          | 34    | 20 | 4 | 10 |         |
| 81  | 1     | 1        | Total | C  | N | O  | 0       |
|     |       |          | 34    | 20 | 4 | 10 |         |
| 81  | 1     | 1        | Total | C  | N | O  | 0       |
|     |       |          | 34    | 20 | 4 | 10 |         |

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| Mol | Chain | Residues | Atoms |    |   |    | AltConf |
|-----|-------|----------|-------|----|---|----|---------|
| 81  | 1     | 1        | Total | C  | N | O  | 0       |
|     |       |          | 34    | 20 | 4 | 10 |         |
| 81  | 1     | 1        | Total | C  | N | O  | 0       |
|     |       |          | 34    | 20 | 4 | 10 |         |
| 81  | A     | 1        | Total | C  | N | O  | 0       |
|     |       |          | 34    | 20 | 4 | 10 |         |
| 81  | A     | 1        | Total | C  | N | O  | 0       |
|     |       |          | 34    | 20 | 4 | 10 |         |
| 81  | A     | 1        | Total | C  | N | O  | 0       |
|     |       |          | 34    | 20 | 4 | 10 |         |
| 81  | A     | 1        | Total | C  | N | O  | 0       |
|     |       |          | 34    | 20 | 4 | 10 |         |
| 81  | AT    | 1        | Total | C  | N | O  | 0       |
|     |       |          | 34    | 20 | 4 | 10 |         |

- Molecule 82 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 82  | b     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 82  | e     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 82  | AH    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 82  | AK    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 82  | AN    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 82  | AP    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 82  | AQ    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |

### 3 Residue-property plots

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

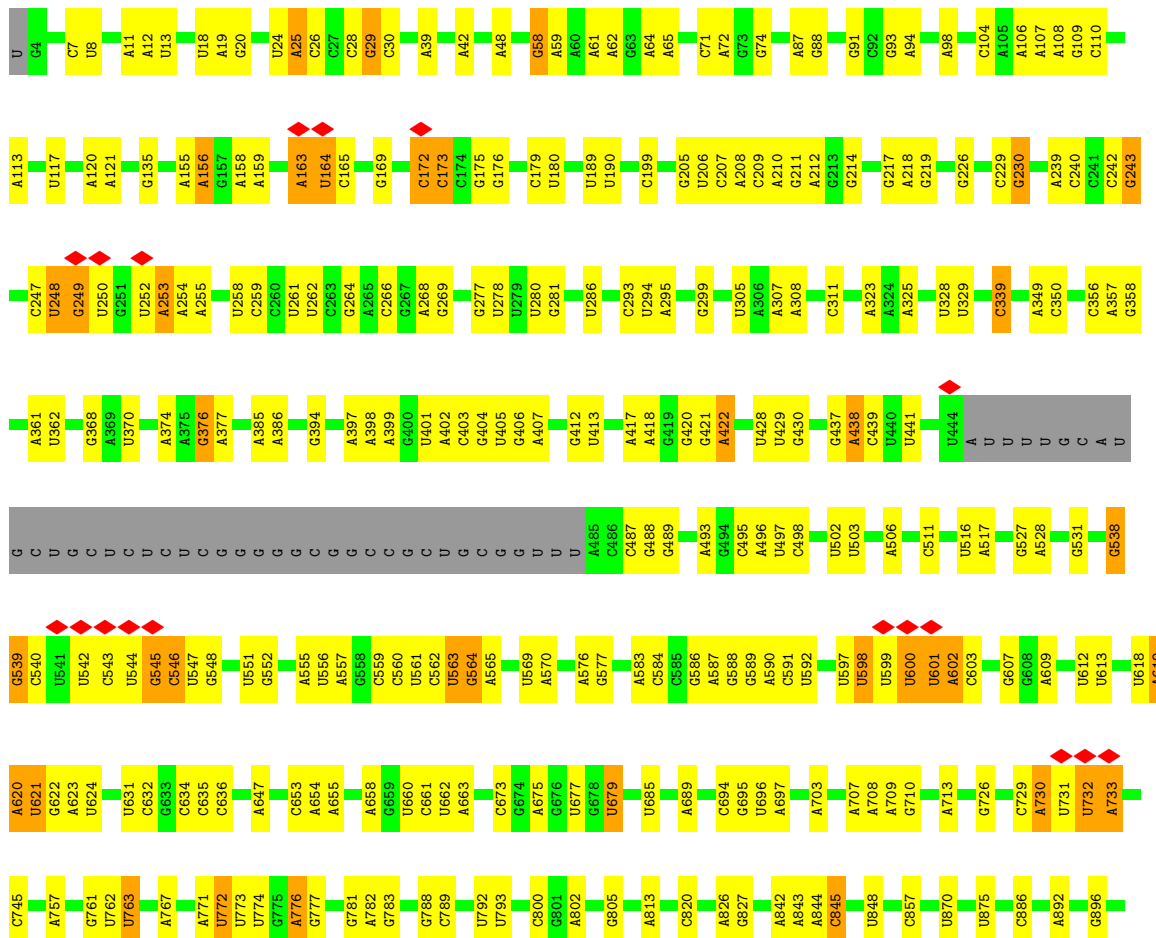
- Molecule 1: 60S ribosomal protein L20

Chain 0: 

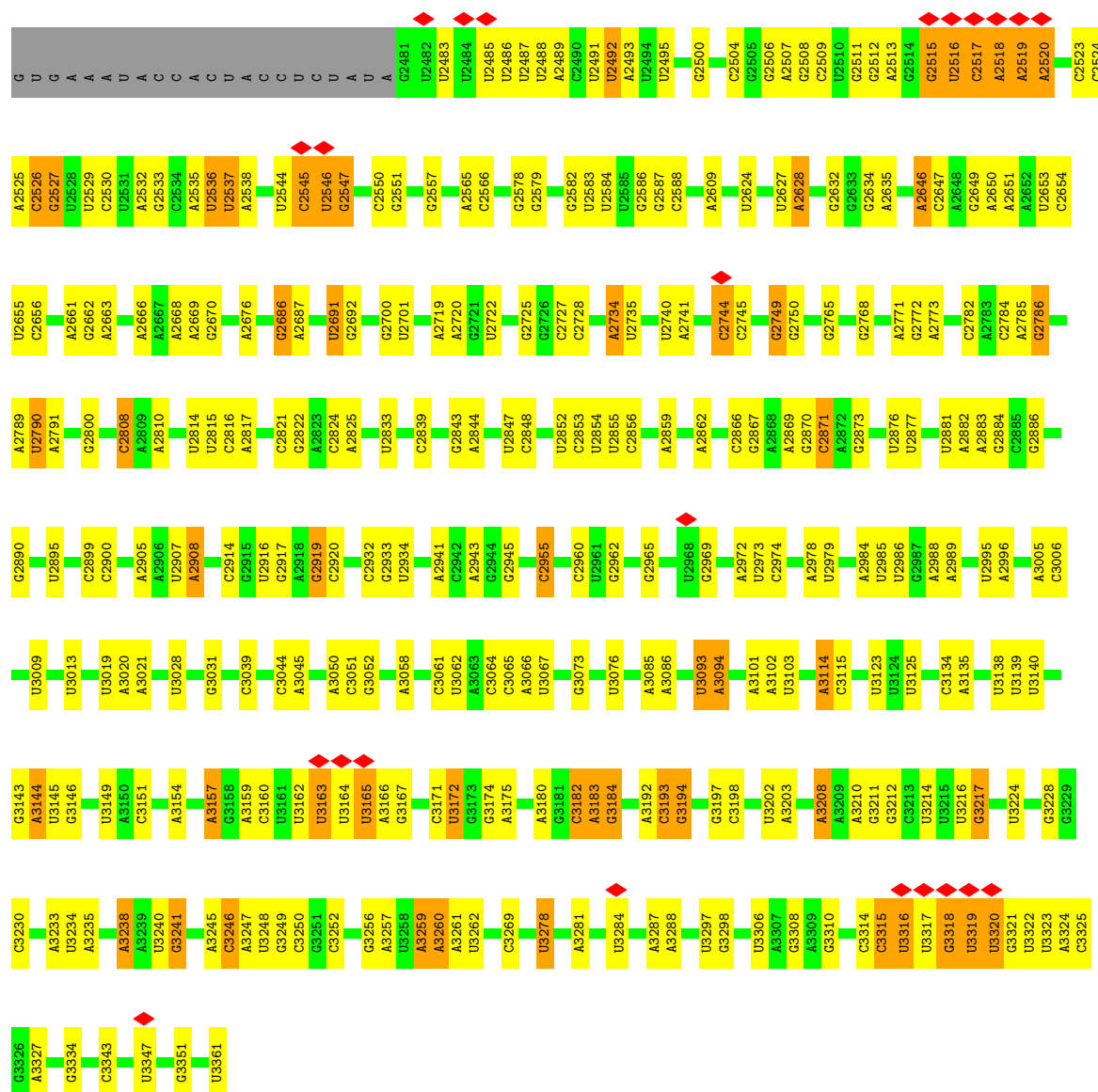


- Molecule 2: 25S rRNA

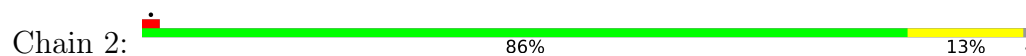
Chain 1: 



|       |       |       |       |       |       |       |       |       |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| C2384 | G2251 | A2130 | G1714 | A1575 | U1451 | A1287 | G1015 | G903  |
| C2385 | A2259 | U2131 | G1715 | A1576 | U1451 | C1288 | G1016 | G904  |
| U2386 | U2260 | A2136 | U1720 | A1585 | A1464 | G1303 | G     | C907  |
| U2389 | G2137 | G2138 | C1721 | A1589 | C1465 | U1305 | U     | A910  |
| A2391 | U2139 | U2140 | G1732 | A1590 | U1466 | U1467 | G     | A911  |
| G2392 | C     | C     | C     | U1591 | U1468 | A1313 | A     | G912  |
| A2397 | U2147 | U2148 | A1746 | C1592 | U1469 | A1314 | A     | A913  |
| C2398 | U2148 | U2149 | G1747 | C1593 | G1470 | A1326 | U     | G919  |
| U2404 | G2149 | U2150 | A1756 | G1594 | A1471 | A1326 | U     | G920  |
| U2405 | U2151 | U2152 | A1757 | A1601 | C1474 | U1330 | A     | A921  |
| U2406 | C2159 | U2153 | U1758 | U1611 | U1475 | U1331 | C     | A922  |
| G2407 | C     | C     | U1759 | U1612 | G1476 | A1339 | U1028 | C923  |
| A2408 | G2163 | U2160 | U1760 | U1613 | A1477 | U1340 | U1029 | C924  |
| C2409 | U2171 | U2161 | G1761 | G1614 | G1483 | U1344 | U1030 | A925  |
| G2413 | G2172 | G1762 | G1763 | A1615 | U1491 | G1345 | A1031 | A926  |
| U2420 | U2182 | C1764 | G1765 | U1616 | U1492 | U1346 | A1032 | G933  |
| A2421 | U2183 | G1766 | U1768 | A1617 | C1493 | U1347 | U1036 | U939  |
| C2422 | G2184 | U1768 | G1774 | U1622 | A1494 | U1348 | A1043 | C940  |
| U2423 | A2185 | G1775 | C1775 | U1625 | U1495 | U1349 | A1044 | C941  |
| G2424 | A2186 | C1776 | G1776 | U1626 | C1504 | C1352 | C1045 | U942  |
| U2425 | U2187 | G1777 | G1777 | U1635 | C1523 | G1353 | A1050 | C944  |
| A2426 | G2188 | G1778 | G1778 | C1636 | A1530 | C1358 | U1058 | U951  |
| U2427 | A2191 | A1782 | A1783 | U1637 | A1531 | A1359 | G1059 | U952  |
| G2428 | A2192 | A1784 | G1792 | A1638 | G1532 | G1376 | A1060 | C955  |
| U2429 | A2201 | A1793 | A1794 | C1639 | A1535 | U1380 | A1061 | U956  |
| A2430 | A2202 | A1795 | A1796 | C1640 | G1543 | G1381 | G1062 | A963  |
| G2431 | U2203 | A1796 | G1803 | U1641 | U1550 | A1382 | U1063 | G964  |
| U2432 | A2206 | G1807 | G1808 | C1653 | U1551 | G1385 | G1068 | C965  |
| A2433 | A2207 | A1809 | A1810 | U1654 | C1552 | C1387 | U1069 | U972  |
| G2434 | A2208 | U1811 | U1812 | G1658 | G1556 | U1395 | U1077 | A976  |
| U2435 | C2209 | G1813 | U1814 | U1662 | U1557 | U1396 | U1078 | U981  |
| A2436 | A2210 | U1815 | U1816 | A1663 | G1558 | G1397 | G1079 | U982  |
| G2437 | A2211 | U1817 | U1818 | G1664 | C1559 | A1415 | A1080 | U983  |
| U2438 | A2222 | A1831 | U1832 | A1679 | U1560 | U1421 | A1081 | U984  |
| A2439 | G2227 | U1833 | U1834 | U1682 | G1562 | U1426 | A1090 | A988  |
| G2440 | U2232 | U1835 | U1836 | U1683 | A1563 | U1432 | U1091 | C989  |
| U2441 | C2235 | U1837 | U1838 | U1684 | U1564 | C1430 | U1092 | G990  |
| A2442 | U2236 | U1839 | U1840 | U1685 | U1565 | U1433 | A1094 | A998  |
| G2443 | A2237 | U1841 | U1842 | C1689 | U1566 | U1434 | A1099 | G1006 |
| U2444 | U2238 | U1843 | U1844 | U1690 | U1567 | U1435 | C     | U1104 |
| A2445 | G2239 | U1845 | U1846 | U1691 | U1568 | C1436 | A     | U1105 |
| G2446 | U2244 | U1847 | U1848 | U1692 | U1569 | U1442 | C     | U1106 |
| C2447 | C2245 | U1849 | U1850 | A1693 | C1569 | G1446 | A1100 | U1107 |
| U2448 | A2246 | U1851 | U1852 | U1713 | U1570 | G1446 | G     | U1108 |
| A2449 | U2247 | U1853 | U1854 |       | G1572 |       |       |       |
| G2450 | C2248 | U1855 | U1856 |       | G1573 |       |       |       |
| U2451 | A2249 | U1857 | U1858 |       | C1574 |       |       |       |
| A2452 | G2249 | U1859 | U1860 |       |       |       |       |       |
| G2453 | U2250 | U1861 | U1862 |       |       |       |       |       |
| U2454 | C2251 | U1863 | U1864 |       |       |       |       |       |
| A2455 | A2252 | U1865 | U1866 |       |       |       |       |       |
| G2456 | U2253 | U1867 | U1868 |       |       |       |       |       |
| U2457 | C2254 | U1869 | U1870 |       |       |       |       |       |
| A2458 | A2255 | U1871 | U1872 |       |       |       |       |       |
| G2459 | U2256 | U1873 | U1874 |       |       |       |       |       |
| U2460 | C2257 | U1875 | U1876 |       |       |       |       |       |
| A2461 | A2258 | U1877 | U1878 |       |       |       |       |       |
| G2462 | U2259 | U1879 | U1880 |       |       |       |       |       |
| U2463 | C2260 | U1881 | U1882 |       |       |       |       |       |
| A2464 | A2261 | U1883 | U1884 |       |       |       |       |       |
| G2465 | U2262 | U1885 | U1886 |       |       |       |       |       |
| U2466 | C2263 | U1887 | U1888 |       |       |       |       |       |
| A2467 | A2264 | U1889 | U1890 |       |       |       |       |       |
| G2468 | U2265 | U1891 | U1892 |       |       |       |       |       |
| U2469 | C2266 | U1893 | U1894 |       |       |       |       |       |
| A2470 | A2267 | U1895 | U1896 |       |       |       |       |       |
| G2471 | U2268 | U1897 | U1898 |       |       |       |       |       |
| U2472 | C2269 | U1899 | U1900 |       |       |       |       |       |
| A2473 | A2270 | U1901 | U1902 |       |       |       |       |       |
| G2474 | U2271 | U1903 | U1904 |       |       |       |       |       |
| U2475 | C2272 | U1905 | U1906 |       |       |       |       |       |
| A2476 | A2273 | U1907 | U1908 |       |       |       |       |       |
| G2477 | U2274 | U1909 | U1910 |       |       |       |       |       |
| U2478 | C2275 | U1911 | U1912 |       |       |       |       |       |
| A2479 | A2276 | U1913 | U1914 |       |       |       |       |       |
| G2480 | U2277 | U1915 | U1916 |       |       |       |       |       |
| U2481 | C2278 | U1917 | U1918 |       |       |       |       |       |
| A2482 | A2279 | U1919 | U1920 |       |       |       |       |       |
| G2483 | U2280 | U1921 | U1922 |       |       |       |       |       |
| U2484 | C2281 | U1923 | U1924 |       |       |       |       |       |
| A2485 | A2282 | U1925 | U1926 |       |       |       |       |       |
| G2486 | U2283 | U1927 | U1928 |       |       |       |       |       |
| U2487 | C2284 | U1929 | U1930 |       |       |       |       |       |
| A2488 | A2285 | U1931 | U1932 |       |       |       |       |       |
| G2489 | U2286 | U1933 | U1934 |       |       |       |       |       |
| U2490 | C2287 | U1935 | U1936 |       |       |       |       |       |
| A2491 | A2288 | U1937 | U1938 |       |       |       |       |       |
| G2492 | U2289 | U1939 | U1940 |       |       |       |       |       |
| U2493 | C2290 | U1941 | U1942 |       |       |       |       |       |
| A2494 | A2291 | U1943 | U1944 |       |       |       |       |       |
| G2495 | U2292 | U1945 | U1946 |       |       |       |       |       |
| U2496 | C2293 | U1947 | U1948 |       |       |       |       |       |
| A2497 | A2294 | U1949 | U1950 |       |       |       |       |       |
| G2498 | U2295 | U1951 | U1952 |       |       |       |       |       |
| U2499 | C2296 | U1953 | U1954 |       |       |       |       |       |
| A2500 | A2297 | U1955 | U1956 |       |       |       |       |       |
| G2501 | U2298 | U1957 | U1958 |       |       |       |       |       |
| U2502 | C2299 | U1959 | U1960 |       |       |       |       |       |
| A2503 | A2300 | U1961 | U1962 |       |       |       |       |       |
| G2504 | U2301 | U1963 | U1964 |       |       |       |       |       |
| U2505 | C2302 | U1965 | U1966 |       |       |       |       |       |
| A2506 | A2303 | U1967 | U1968 |       |       |       |       |       |
| G2507 | U2304 | U1969 | U1970 |       |       |       |       |       |
| U2508 | C2305 | U1971 | U1972 |       |       |       |       |       |
| A2509 | A2306 | U1973 | U1974 |       |       |       |       |       |
| G2510 | U2307 | U1975 | U1976 |       |       |       |       |       |
| U2511 | C2308 | U1977 | U1978 |       |       |       |       |       |
| A2512 | A2309 | U1979 | U1980 |       |       |       |       |       |
| G2513 | U2309 | U1981 | U1982 |       |       |       |       |       |
| U2514 | C2310 | U1983 | U1984 |       |       |       |       |       |
| A2515 | A2311 | U1985 | U1986 |       |       |       |       |       |
| G2516 | U2312 | U1987 | U1988 |       |       |       |       |       |
| U2517 | C2313 | U1989 | U1990 |       |       |       |       |       |
| A2518 | A2314 | U1991 | U1992 |       |       |       |       |       |
| G2519 | U2315 | U1993 | U1994 |       |       |       |       |       |
| U2520 | C2316 | U1995 | U1996 |       |       |       |       |       |
| A2521 | A2317 | U1997 | U1998 |       |       |       |       |       |
| G2522 | U2318 | U1999 | U2000 |       |       |       |       |       |
| U2523 | C2319 | U2001 | U2002 |       |       |       |       |       |
| A2524 | A2320 | U2003 | U2004 |       |       |       |       |       |
| G2525 | U2321 | U2005 | U2006 |       |       |       |       |       |
| U2526 | C2322 | U2007 | U2008 |       |       |       |       |       |
| A2527 | A2323 | U2009 | U2010 |       |       |       |       |       |
| G2528 | U2324 | U2011 | U2012 |       |       |       |       |       |
| U2529 | C2325 | U2013 | U2014 |       |       |       |       |       |
| A2530 | A2326 | U2015 | U2016 |       |       |       |       |       |
| G2531 | U2327 | U2017 | U2018 |       |       |       |       |       |
| U2532 | C2328 | U2019 | U2020 |       |       |       |       |       |
| A2533 | A2329 | U2021 | U2022 |       |       |       |       |       |
| G2534 | U2330 | U2023 | U2024 |       |       |       |       |       |
| U2535 | C2331 | U2025 | U2026 |       |       |       |       |       |
| A2536 | A2332 | U2027 | U2028 |       |       |       |       |       |
| G2537 | U2333 | U2029 | U2030 |       |       |       |       |       |
| U2538 | C2334 | U2031 | U2032 |       |       |       |       |       |
| A2539 | A2335 | U2033 | U2034 |       |       |       |       |       |
| G2540 | U2336 | U2035 | U2036 |       |       |       |       |       |
| U2541 | C2337 | U2037 | U2038 |       |       |       |       |       |
| A2542 | A2338 | U2039 | U2040 |       |       |       |       |       |
| G2543 | U2339 | U2041 | U2042 |       |       |       |       |       |
| U2544 | C2340 | U2043 | U2044 |       |       |       |       |       |
| A2545 | A2341 | U2045 | U2046 |       |       |       |       |       |
| G2546 | U2342 | U2047 | U2048 |       |       |       |       |       |
| U2547 | C2343 | U2049 | U2050 |       |       |       |       |       |
| A2548 | A2344 | U2051 | U2052 |       |       |       |       |       |
| G2549 | U2345 | U2053 | U2054 |       |       |       |       |       |
| U2550 | C2346 | U2055 | U2056 |       |       |       |       |       |
| A2551 | A2347 | U2057 | U2058 |       |       |       |       |       |
| G2552 | U2348 | U2059 | U2060 |       |       |       |       |       |
| U2553 | C2349 | U2061 | U2062 |       |       |       |       |       |
| A2554 | A2350 | U2063 | U2064 |       |       |       |       |       |
| G2555 | U2351 | U2065 | U2066 |       |       |       |       |       |
| U2556 | C2352 | U2067 | U2068 |       |       |       |       |       |
| A2557 | A2353 | U2069 | U2070 |       |       |       |       |       |
| G2558 | U2354 | U2071 | U2072 |       |       |       |       |       |
| U2559 | C2355 | U2073 | U2074 |       |       |       |       |       |
| A2560 | A2356 | U2075 | U2076 |       |       |       |       |       |
| G2561 | U2357 | U2077 | U2078 |       |       |       |       |       |
| U2562 | C2358 | U2079 | U2080 |       |       |       |       |       |
| A2563 | A2359 | U2081 | U2082 |       |       |       |       |       |
| G2564 | U2360 | U2083 | U2084 |       |       |       |       |       |
| U2565 | C2361 | U2085 | U2086 |       |       |       |       |       |
| A2566 | A2362 | U2087 | U2088 |       |       |       |       |       |
| G2567 | U2363 | U2089 | U2090 |       |       |       |       |       |
| U2568 | C2364 | U2091 | U2092 |       |       |       |       |       |
| A2569 | A2365 | U2093 | U2094 |       |       |       |       |       |
| G2570 | U2366 | U2095 | U2096 |       |       |       |       |       |
| U2571 | C2367 | U2097 | U2098 |       |       |       |       |       |
| A2572 | A2368 | U2099 | U2100 |       |       |       |       |       |
| G2573 | U2369 | U2101 | U2102 |       |       |       |       |       |
| U2574 | C2370 | U2103 | U2104 |       |       |       |       |       |
| A2575 | A2371 | U2105 | U2106 |       |       |       |       |       |
| G2576 | U2372 | U2107 | U2108 |       |       |       |       |       |
| U2577 | C2373 | U2109 | U2110 |       |       |       |       |       |
| A2578 | A2374 | U2111 | U2112 |       |       |       |       |       |
| G2579 | U2375 | U2113 | U2114 |       |       |       |       |       |
| U2580 | C2376 | U2115 | U2116 |       |       |       |       |       |
| A2581 | A2377 | U2117 | U2118 |       |       |       |       |       |
| G2582 | U2378 | U2119 | U2120 |       |       |       |       |       |
| U2583 | C2379 | U2121 | U2122 |       |       |       |       |       |



• Molecule 3: 60S ribosomal protein L21-A

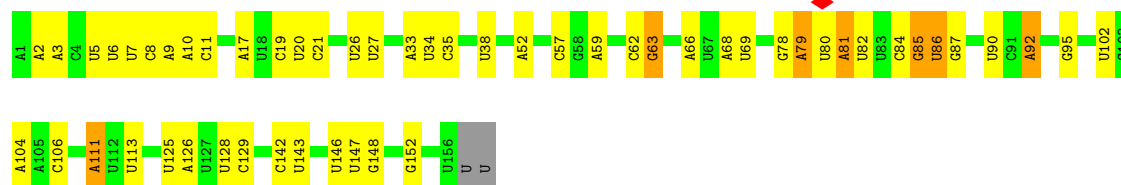


• Molecule 4: 5S rRNA



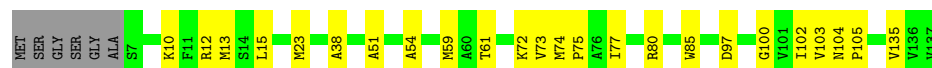
• Molecule 5: 5.8S rRNA

Chain 4:  65% 30%



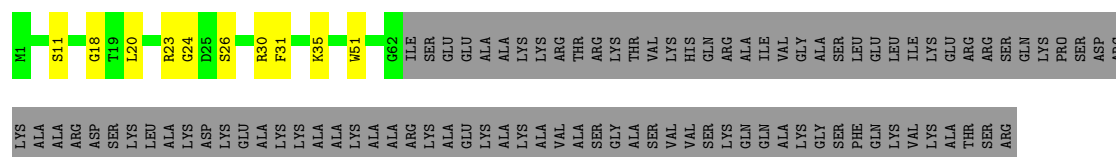
- Molecule 6: 60S ribosomal protein L23-A

Chain 6:  78% 18%



- Molecule 7: 60S ribosomal protein L24-A

Chain 7:  34% 6% 60%



- Molecule 8: 60S ribosomal protein L25

Chain 8:  73% 11% 16%



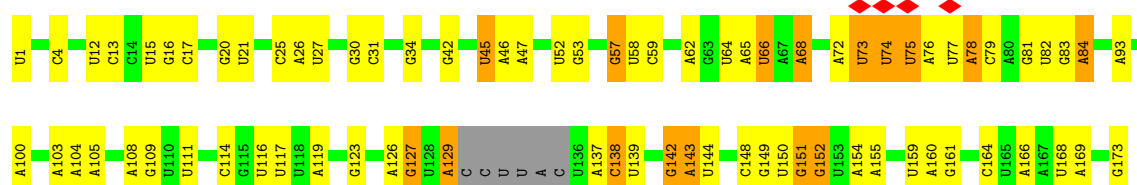
- Molecule 9: Ribosomal protein L24

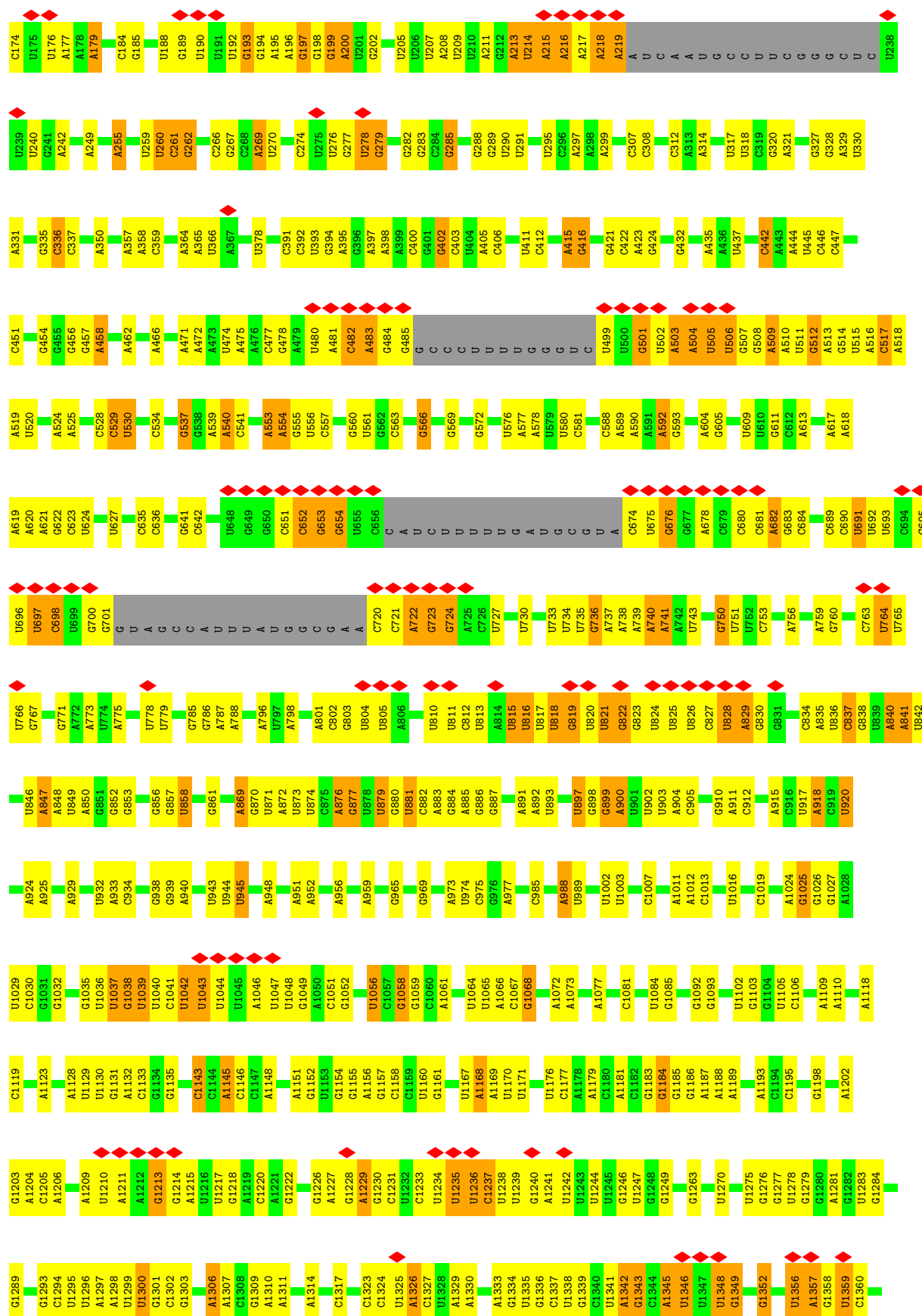
Chain 9:  88% 10%

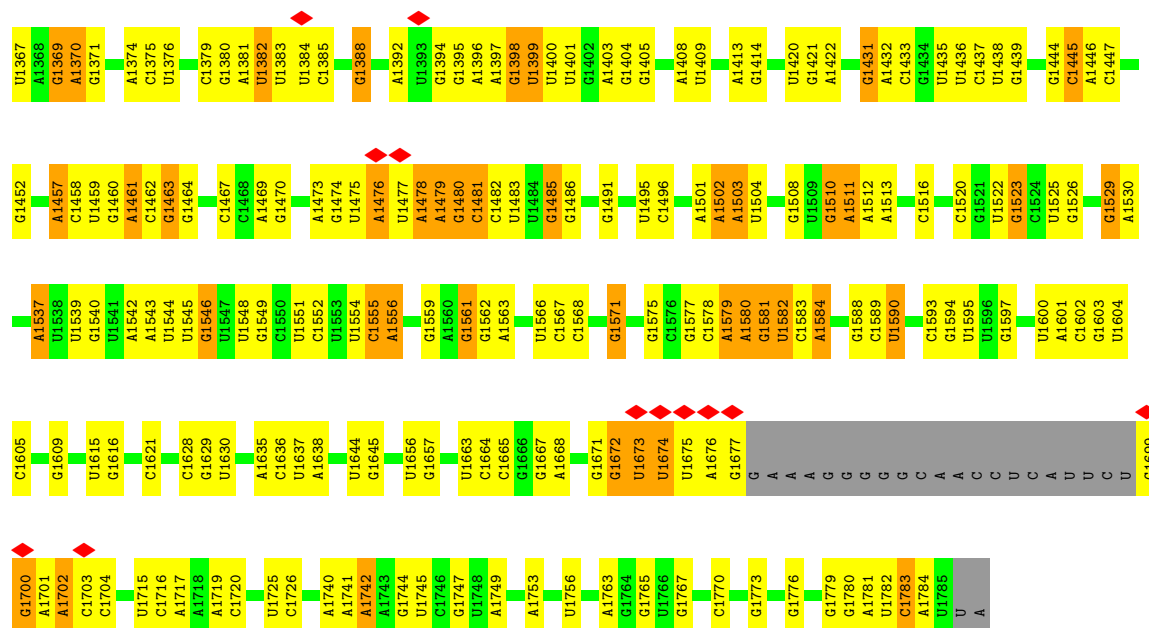


- Molecule 10: 18S rRNA

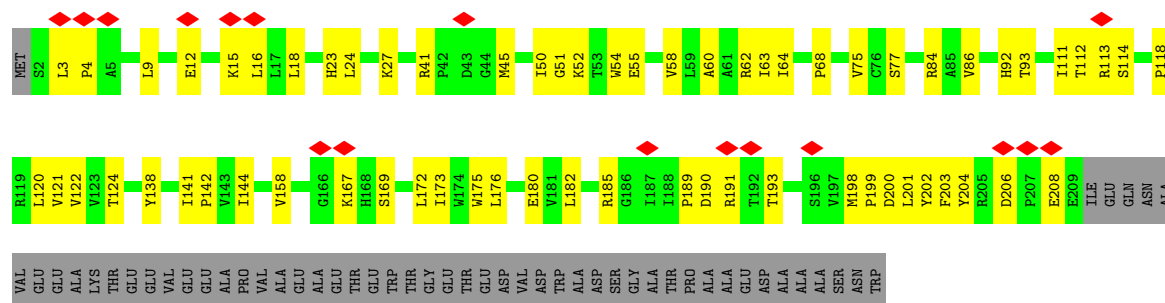
Chain A:  7% 48% 37% 10% 5%



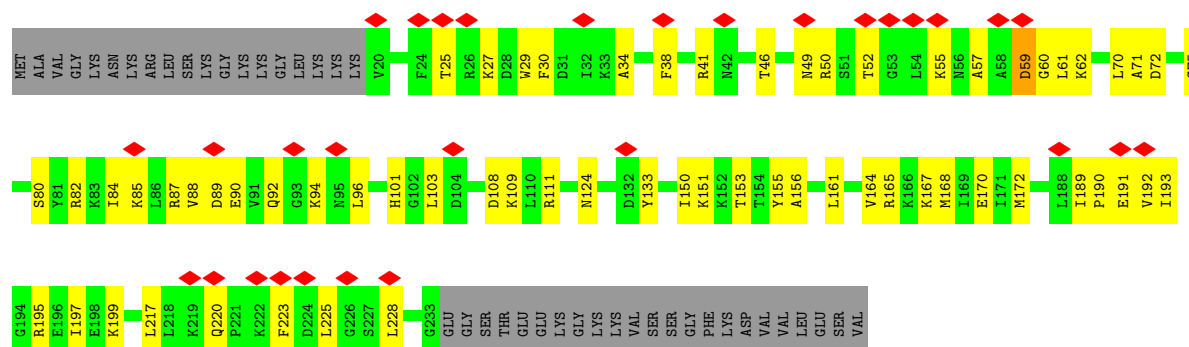




• Molecule 11: 40S ribosomal protein S0

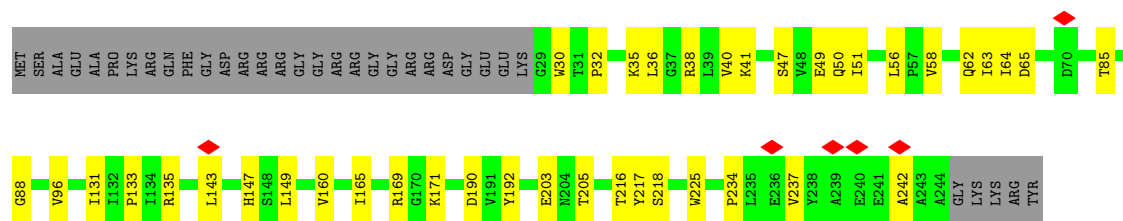


• Molecule 12: 40S ribosomal protein S1

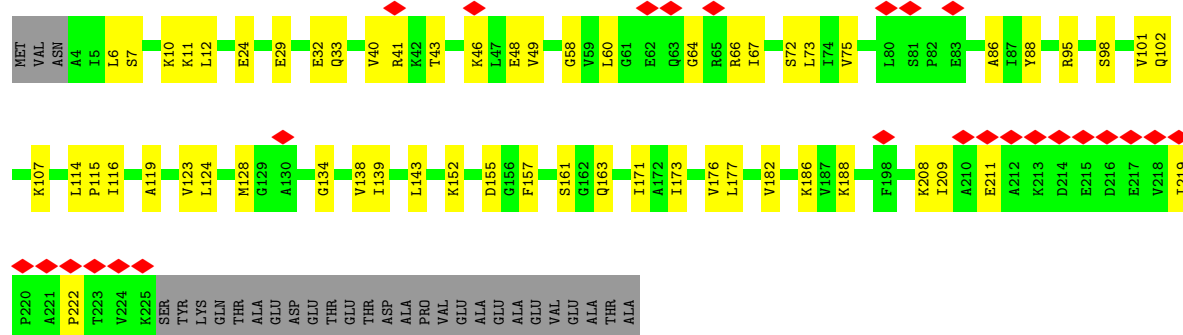


• Molecule 13: Ribosomal protein S5

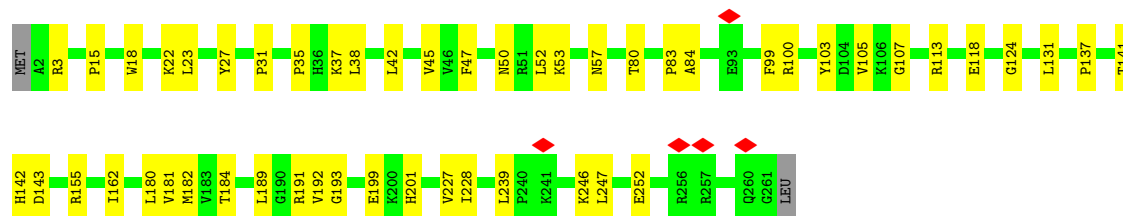
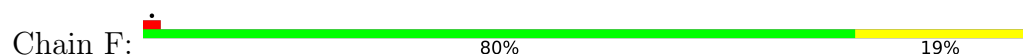




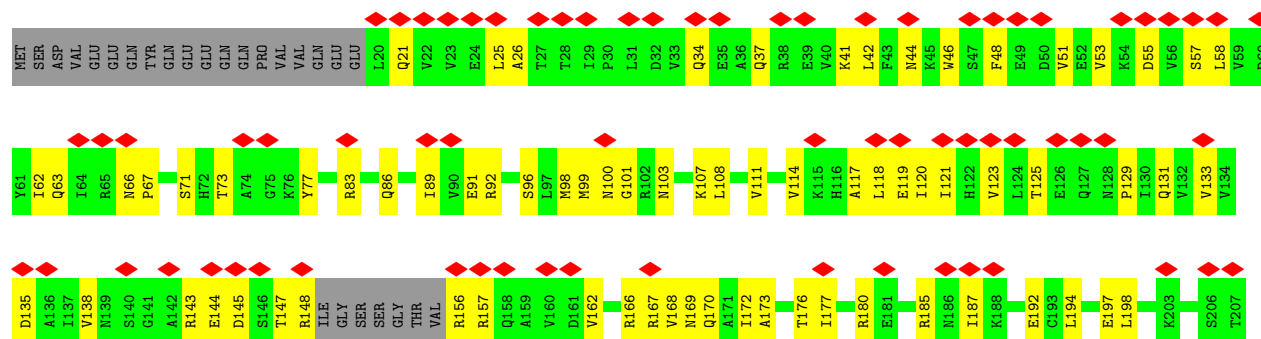
• Molecule 14: Ribosomal protein S3



• Molecule 15: 40S ribosomal protein S4

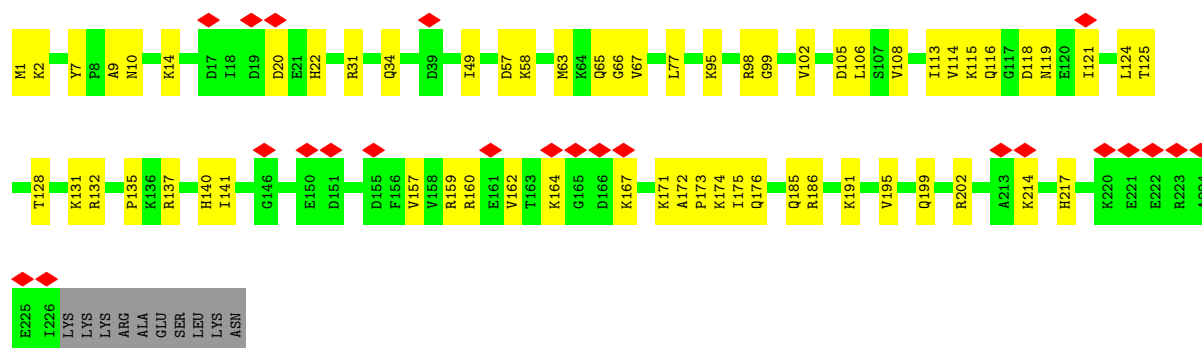


• Molecule 16: Ribosomal protein S7

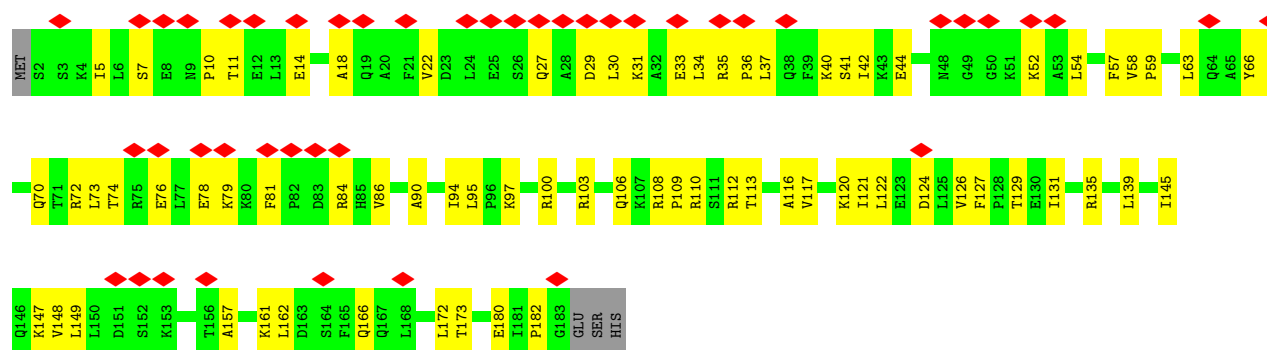




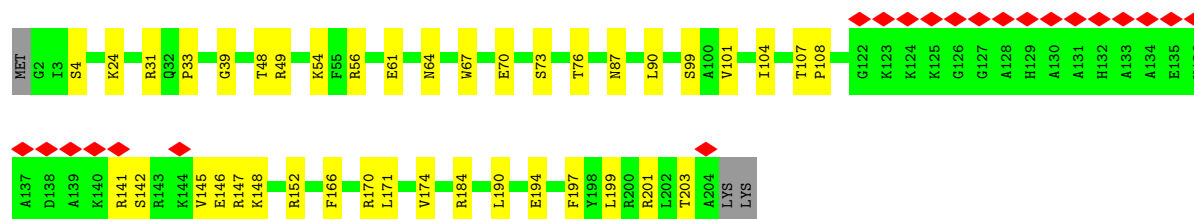
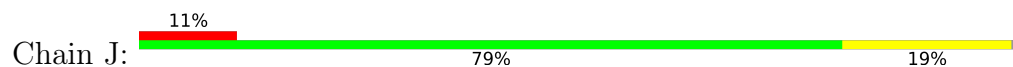
• Molecule 17: 40S ribosomal protein S6



• Molecule 18: 40S ribosomal protein S7

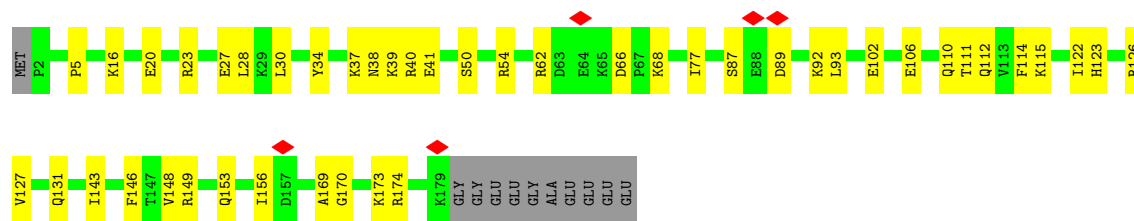


• Molecule 19: 40S ribosomal protein S8

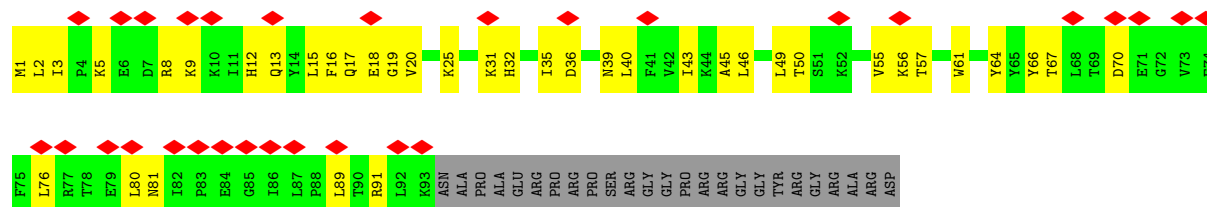


• Molecule 20: Ribosomal protein S4

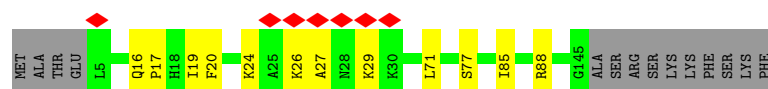
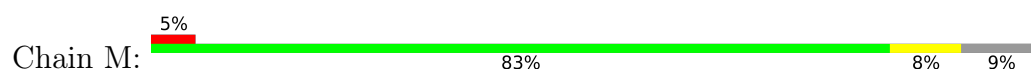




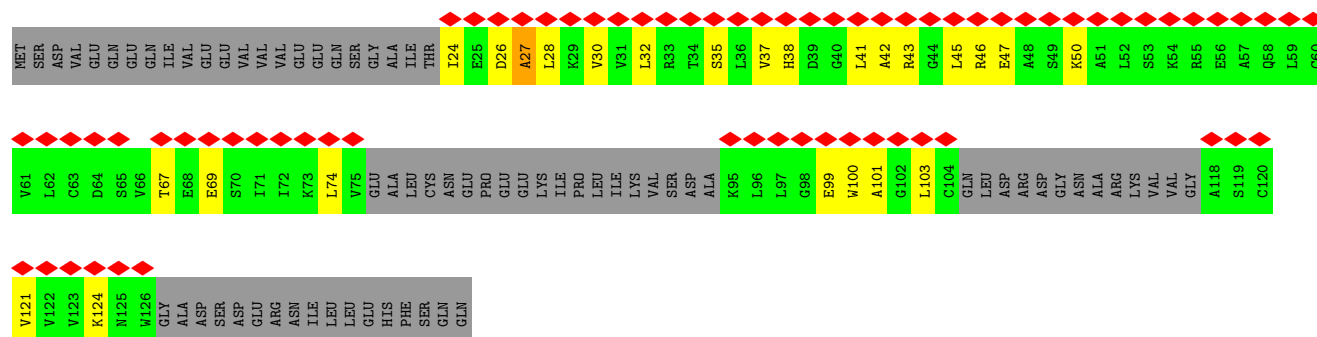
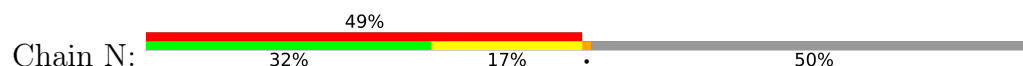
• Molecule 21: 40S ribosomal protein S10-A



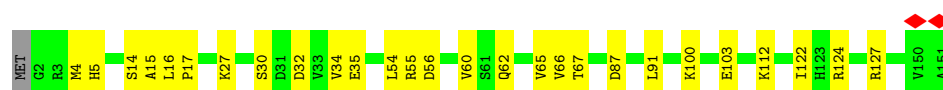
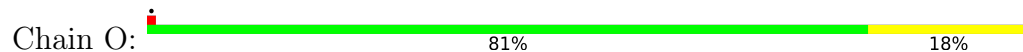
• Molecule 22: 40S ribosomal protein S11A



• Molecule 23: 40S ribosomal protein S12

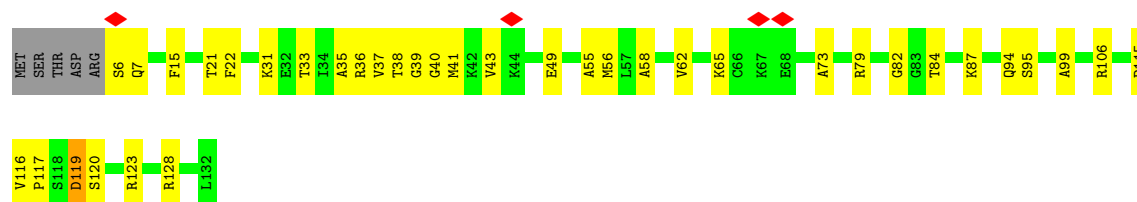


• Molecule 24: 40S ribosomal protein S13



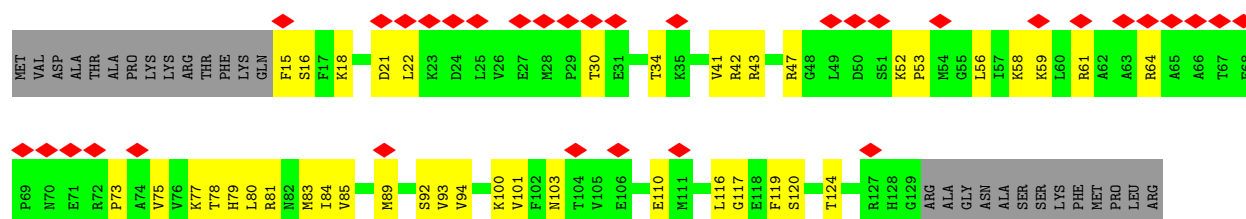
• Molecule 25: 40S ribosomal protein S14-A

Chain P: 



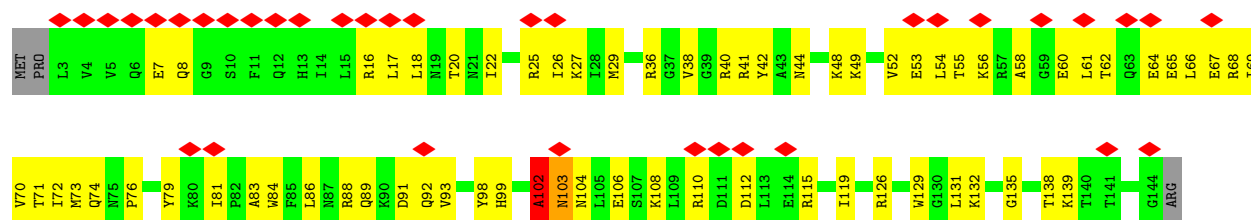
- Molecule 26: 40S ribosomal protein S15

Chain Q: 



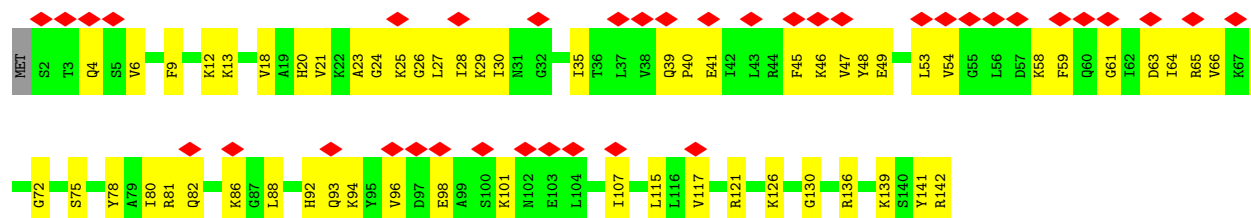
- Molecule 27: 40S ribosomal protein S18-B

Chain T: 



- Molecule 28: 40S ribosomal protein S16

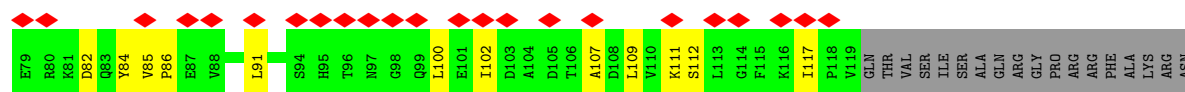
Chain R: 



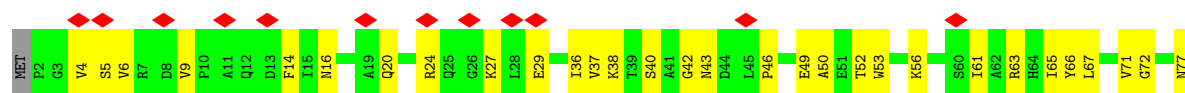
- Molecule 29: 40S ribosomal protein S17-B

Chain S: 

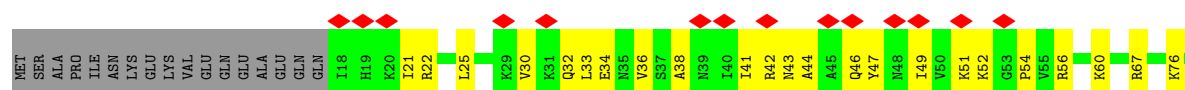




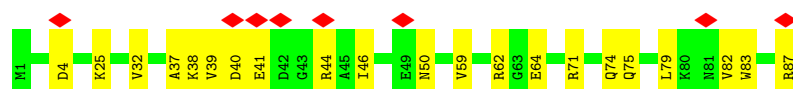
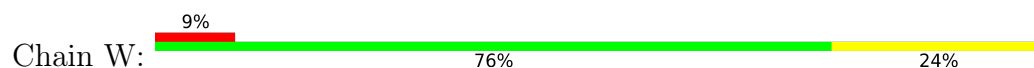
• Molecule 30: 40S ribosomal protein S19-A



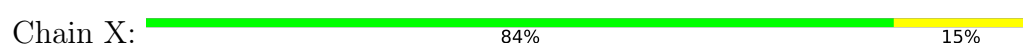
• Molecule 31: Ribosomal protein S10



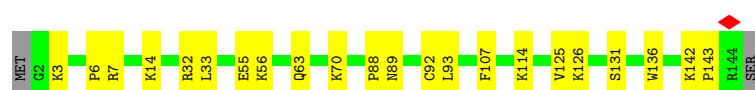
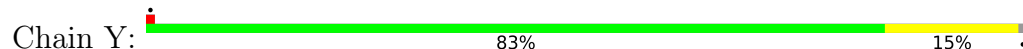
• Molecule 32: 40S ribosomal protein S21



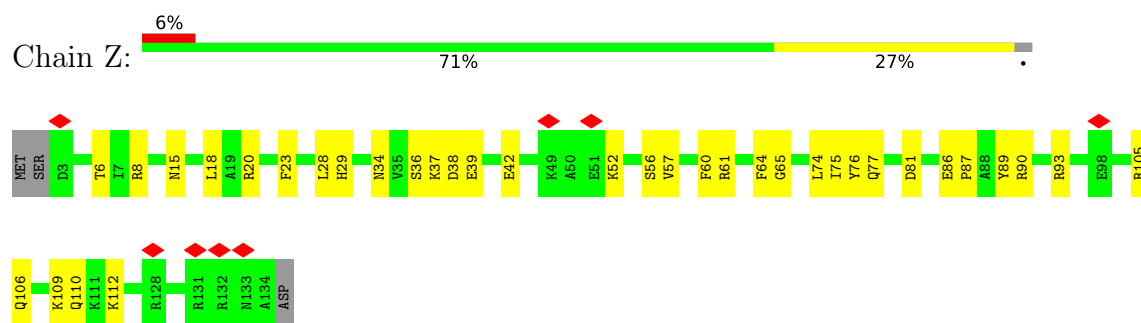
• Molecule 33: 40S ribosomal protein S22-A



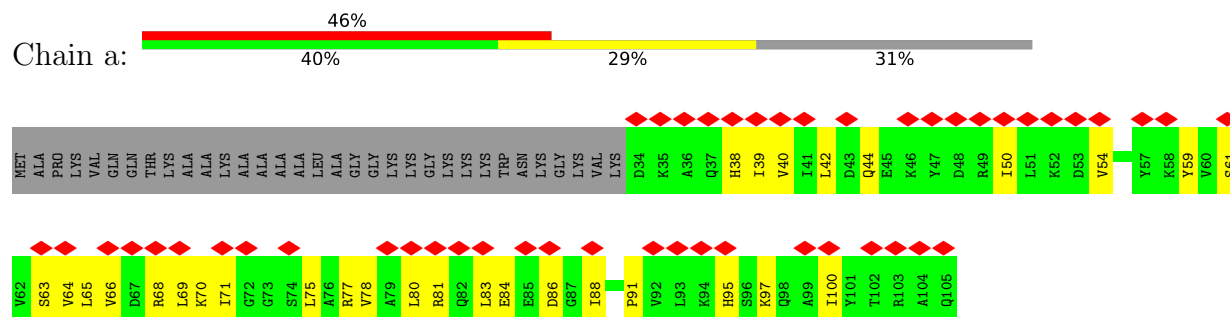
• Molecule 34: Ribosomal protein S23 (S12)



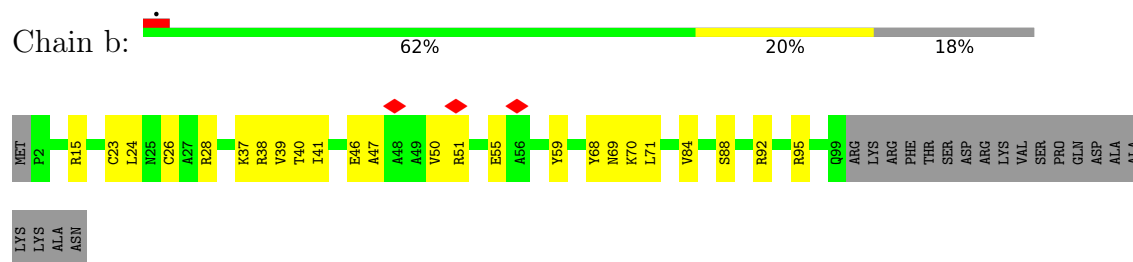
• Molecule 35: 40S ribosomal protein S24



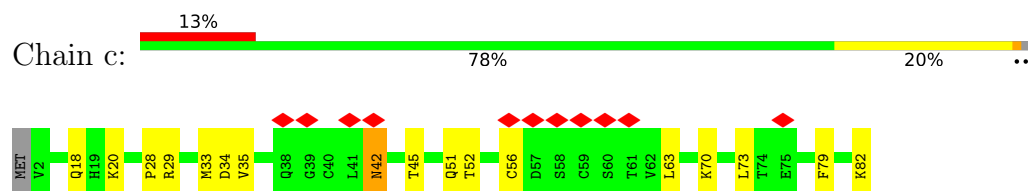
- Molecule 36: 40S ribosomal protein S25



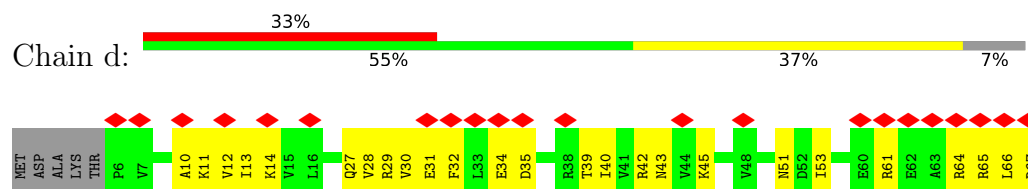
- Molecule 37: 40S ribosomal protein S26



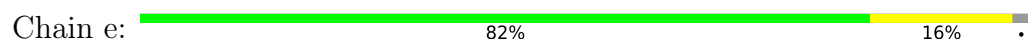
- Molecule 38: 40S ribosomal protein S27



- Molecule 39: 40S ribosomal protein S28-B



- Molecule 40: 40S ribosomal protein S29A

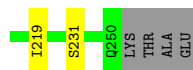






- Molecule 44: 60S ribosomal protein L2-B

Chain j: 85% 13%



- Molecule 45: 60S ribosomal protein L3

Chain k: 86% 14%



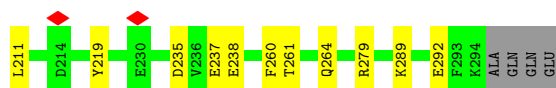
- Molecule 46: 60S ribosomal protein L4-B

Chain l: 90% 9%



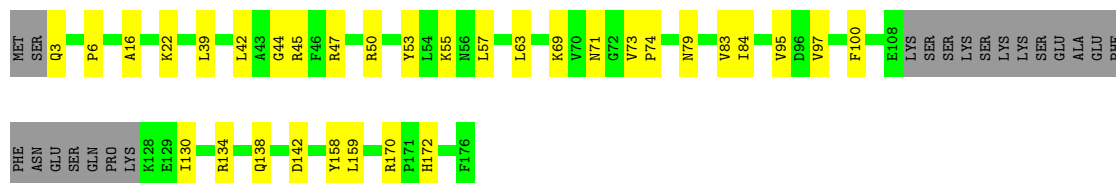
- Molecule 47: 60S ribosomal protein L5

Chain m: 84% 14%



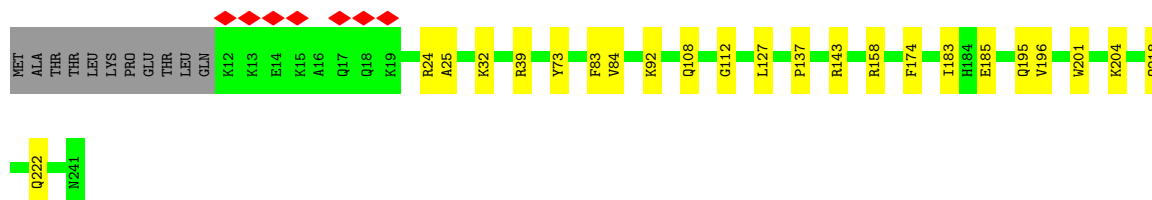
- Molecule 48: 60S ribosomal protein L6

Chain n:  70% 18% 12%



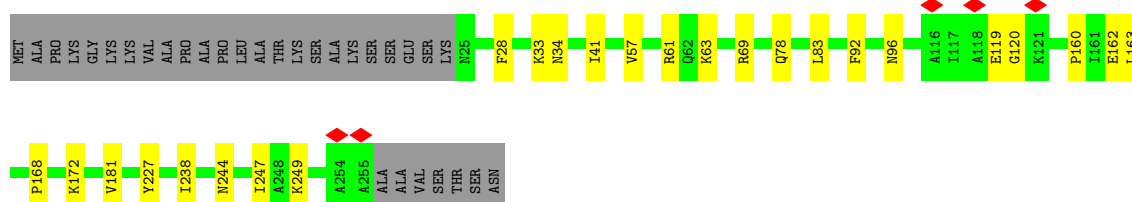
- Molecule 49: 60S ribosomal protein L7-A

Chain o:  86% 10% 5%



- Molecule 50: 60S ribosomal protein L8

Chain p:  79% 10% 12%



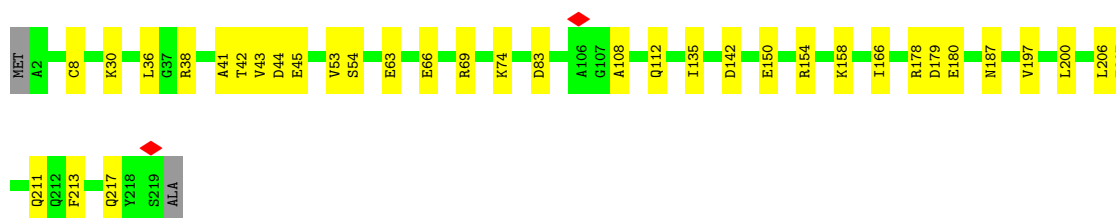
- Molecule 51: 60S ribosomal protein L9-B

Chain q:  85% 14% .

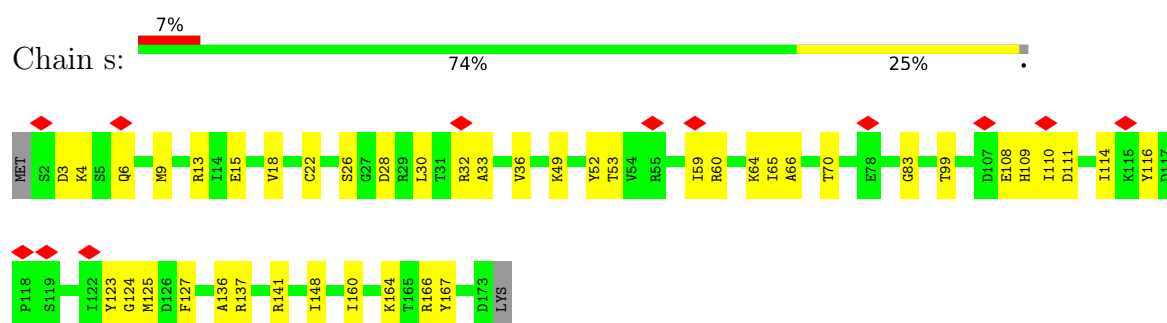


- Molecule 52: 60S ribosomal protein L10

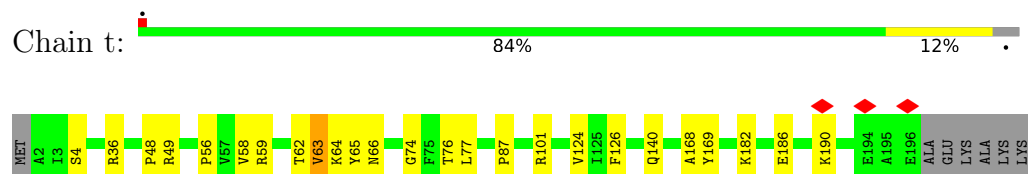
Chain r:  83% 16% .



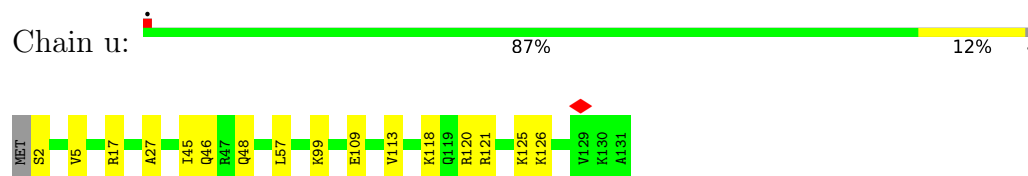
- Molecule 53: 60S ribosomal protein L11-B



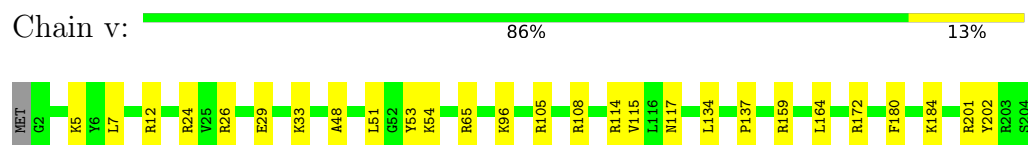
- Molecule 54: 60S ribosomal protein L13



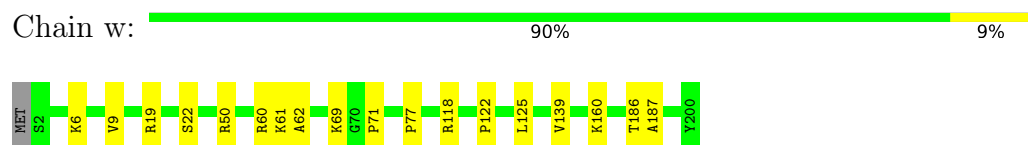
- Molecule 55: 60S ribosomal protein L14-B



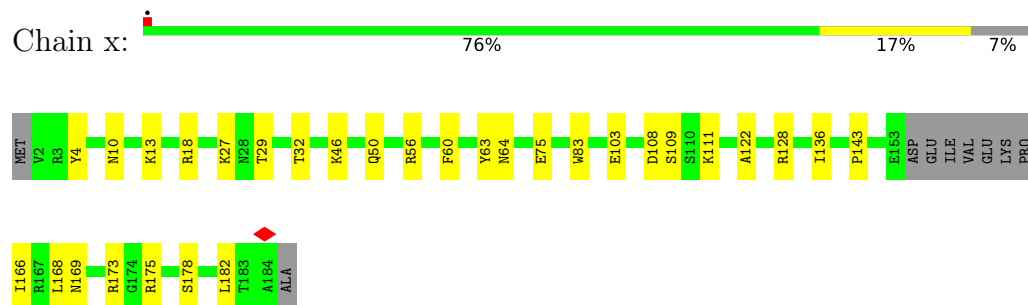
- Molecule 56: 60S ribosomal protein L15-A



- Molecule 57: Ribosomal protein L13

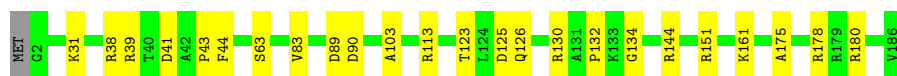


- Molecule 58: Ribosomal protein L22



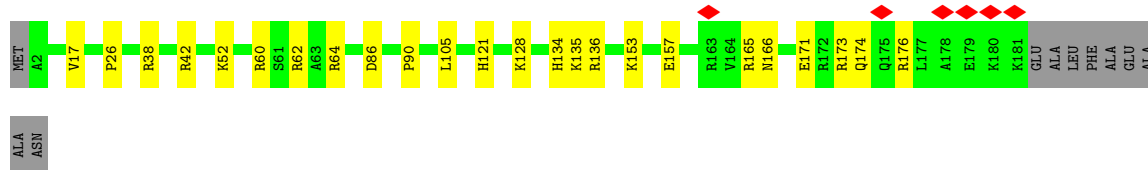
- Molecule 59: 60S ribosomal protein L18-A

Chain y:  87% 13%



- Molecule 60: 60S ribosomal protein L19-A

Chain z:  82% 13% 5%



- Molecule 61: 60S ribosomal protein L27

Chain AA:  82% 17%



- Molecule 62: 60S ribosomal protein L28

Chain AB:  85% 14%



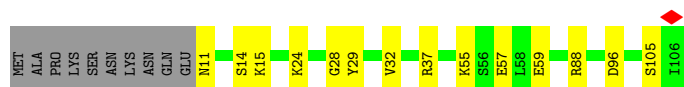
- Molecule 63: 60S ribosomal protein L29

Chain AC:  86% 10% 5%



- Molecule 64: 60S ribosomal protein L30

Chain AD:  77% 13% 9%



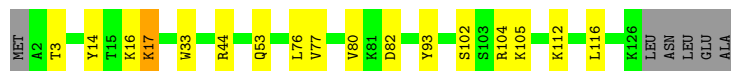
- Molecule 65: 60S ribosomal protein L31-B

Chain AE:  82% 14%



- Molecule 66: 60S ribosomal protein L32

Chain AF: 82% 12% 5%



- Molecule 67: 60S ribosomal protein L33-A

Chain AG: 86% 13% 1%



- Molecule 68: 60S ribosomal protein L34-B

Chain AH: 80% 11% 8%



- Molecule 69: Ribosomal protein L29

Chain AI: 84% 15% 1%



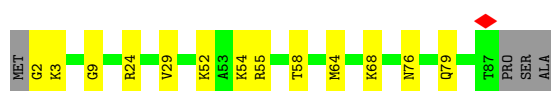
- Molecule 70: 60S ribosomal protein L36

Chain AJ: 80% 18% 2%

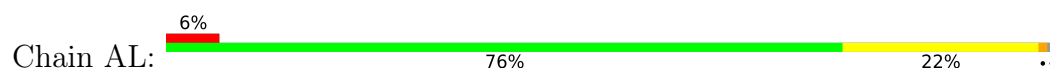


- Molecule 71: 60S ribosomal protein L37-B

Chain AK: 81% 14% 5%



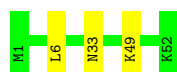
- Molecule 72: 60S ribosomal protein L38



- Molecule 73: 60S ribosomal protein L39



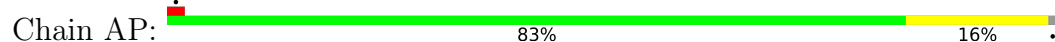
- Molecule 74: 60S ribosomal protein L40-B



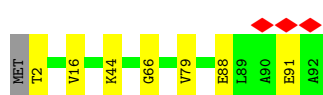
- Molecule 75: 60S ribosomal protein L41



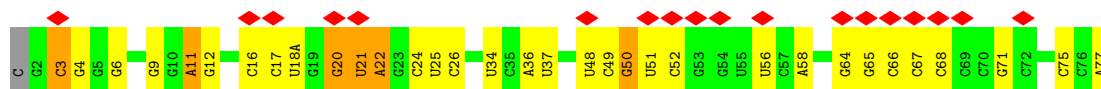
- Molecule 76: 60S ribosomal protein L42-B



- Molecule 77: 60S ribosomal protein L43-A



- Molecule 78: tRNA



Chain AT: 



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 44555                                   | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TITAN KRIOS                         | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 29.7                                    | Depositor |
| Minimum defocus (nm)                 | 200                                     | Depositor |
| Maximum defocus (nm)                 | 1200                                    | Depositor |
| Magnification                        | Not provided                            |           |
| Image detector                       | FEI FALCON IV (4k x 4k)                 | Depositor |
| Maximum map value                    | 1.915                                   | Depositor |
| Minimum map value                    | -0.740                                  | Depositor |
| Average map value                    | 0.002                                   | Depositor |
| Map value standard deviation         | 0.055                                   | Depositor |
| Recommended contour level            | 0.168                                   | Depositor |
| Map size (Å)                         | 510.3, 510.3, 510.3                     | wwPDB     |
| Map dimensions                       | 700, 700, 700                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 0.729, 0.729, 0.729                     | Depositor |

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: IAS, OMC, SPK, ZN, MLZ, GET, OMG

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

| Mol | Chain | Bond lengths |             | Bond angles |             |
|-----|-------|--------------|-------------|-------------|-------------|
|     |       | RMSZ         | $\# Z  > 5$ | RMSZ        | $\# Z  > 5$ |
| 1   | 0     | 0.25         | 0/1483      | 0.40        | 0/1997      |
| 2   | 1     | 0.32         | 0/73296     | 0.36        | 0/114257    |
| 3   | 2     | 0.26         | 0/1305      | 0.39        | 0/1749      |
| 4   | 3     | 0.26         | 0/2884      | 0.29        | 0/4492      |
| 5   | 4     | 0.31         | 0/3702      | 0.34        | 0/5764      |
| 6   | 6     | 0.25         | 0/994       | 0.41        | 0/1339      |
| 7   | 7     | 0.25         | 0/528       | 0.41        | 0/701       |
| 8   | 8     | 0.25         | 0/976       | 0.39        | 0/1319      |
| 9   | 9     | 0.24         | 0/990       | 0.40        | 0/1322      |
| 10  | A     | 0.24         | 0/40362     | 0.35        | 0/62888     |
| 11  | B     | 0.20         | 0/1666      | 0.41        | 0/2273      |
| 12  | C     | 0.17         | 0/1750      | 0.41        | 0/2354      |
| 13  | D     | 0.20         | 0/1648      | 0.36        | 0/2237      |
| 14  | E     | 0.18         | 0/1725      | 0.38        | 0/2316      |
| 15  | F     | 0.20         | 0/2096      | 0.38        | 0/2822      |
| 16  | G     | 0.18         | 0/1588      | 0.42        | 0/2139      |
| 17  | H     | 0.18         | 0/1845      | 0.35        | 0/2464      |
| 18  | I     | 0.19         | 0/1490      | 0.40        | 0/2004      |
| 19  | J     | 0.21         | 0/1606      | 0.36        | 0/2150      |
| 20  | K     | 0.20         | 0/1478      | 0.39        | 0/1978      |
| 21  | L     | 0.19         | 0/801       | 0.41        | 0/1081      |
| 22  | M     | 0.22         | 0/1154      | 0.40        | 0/1553      |
| 23  | N     | 0.19         | 0/541       | 0.52        | 0/726       |
| 24  | O     | 0.20         | 0/1210      | 0.32        | 0/1631      |
| 25  | P     | 0.16         | 0/944       | 0.34        | 0/1265      |
| 26  | Q     | 0.17         | 0/924       | 0.40        | 0/1243      |
| 27  | T     | 0.18         | 0/1186      | 0.43        | 0/1590      |
| 28  | R     | 0.18         | 0/1120      | 0.46        | 0/1500      |
| 29  | S     | 0.17         | 0/966       | 0.40        | 0/1295      |
| 30  | U     | 0.17         | 0/1120      | 0.36        | 0/1508      |
| 31  | V     | 0.17         | 0/800       | 0.42        | 0/1082      |
| 32  | W     | 0.19         | 0/683       | 0.38        | 0/918       |

| Mol | Chain | Bond lengths |         | Bond angles |              |
|-----|-------|--------------|---------|-------------|--------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5      |
| 33  | X     | 0.23         | 0/1049  | 0.37        | 0/1412       |
| 34  | Y     | 0.23         | 0/1128  | 0.41        | 0/1505       |
| 35  | Z     | 0.17         | 0/1086  | 0.40        | 0/1447       |
| 36  | a     | 0.19         | 0/585   | 0.49        | 0/789        |
| 37  | b     | 0.20         | 0/791   | 0.39        | 0/1060       |
| 38  | c     | 0.18         | 0/624   | 0.38        | 0/843        |
| 39  | d     | 0.16         | 0/489   | 0.41        | 0/654        |
| 40  | e     | 0.17         | 0/466   | 0.37        | 0/620        |
| 41  | f     | 0.19         | 0/469   | 0.39        | 0/626        |
| 42  | g     | 0.23         | 0/575   | 0.66        | 3/760 (0.4%) |
| 43  | h     | 0.15         | 0/1898  | 0.39        | 0/2584       |
| 44  | j     | 0.29         | 0/1931  | 0.43        | 0/2592       |
| 45  | k     | 0.27         | 0/3156  | 0.41        | 0/4246       |
| 46  | l     | 0.25         | 0/2799  | 0.41        | 0/3777       |
| 47  | m     | 0.21         | 0/2447  | 0.37        | 0/3294       |
| 48  | n     | 0.23         | 0/1258  | 0.39        | 0/1696       |
| 49  | o     | 0.25         | 0/1896  | 0.42        | 0/2544       |
| 50  | p     | 0.25         | 0/1825  | 0.40        | 0/2458       |
| 51  | q     | 0.23         | 0/1528  | 0.37        | 0/2055       |
| 52  | r     | 0.22         | 0/1795  | 0.34        | 0/2411       |
| 53  | s     | 0.19         | 0/1404  | 0.38        | 0/1880       |
| 54  | t     | 0.26         | 0/1600  | 0.43        | 0/2147       |
| 55  | u     | 0.25         | 0/1044  | 0.41        | 0/1407       |
| 56  | v     | 0.28         | 0/1753  | 0.41        | 0/2347       |
| 57  | w     | 0.26         | 0/1620  | 0.39        | 0/2167       |
| 58  | x     | 0.26         | 0/1398  | 0.39        | 0/1879       |
| 59  | y     | 0.26         | 0/1511  | 0.44        | 0/2022       |
| 60  | z     | 0.24         | 0/1492  | 0.40        | 0/1983       |
| 61  | AA    | 0.23         | 0/1112  | 0.32        | 0/1488       |
| 62  | AB    | 0.26         | 0/1199  | 0.41        | 0/1607       |
| 63  | AC    | 0.23         | 0/502   | 0.36        | 0/666        |
| 64  | AD    | 0.21         | 0/738   | 0.31        | 0/994        |
| 65  | AE    | 0.24         | 0/894   | 0.38        | 0/1201       |
| 66  | AF    | 0.26         | 0/1039  | 0.41        | 0/1390       |
| 67  | AG    | 0.27         | 0/895   | 0.36        | 0/1201       |
| 68  | AH    | 0.25         | 0/934   | 0.42        | 0/1242       |
| 69  | AI    | 0.24         | 0/1004  | 0.43        | 0/1337       |
| 70  | AJ    | 0.23         | 0/772   | 0.36        | 0/1023       |
| 71  | AK    | 0.30         | 0/690   | 0.48        | 0/916        |
| 72  | AL    | 0.24         | 0/632   | 0.38        | 0/842        |
| 73  | AM    | 0.24         | 0/458   | 0.37        | 0/609        |
| 74  | AN    | 0.22         | 0/436   | 0.35        | 0/577        |
| 75  | AO    | 0.14         | 0/237   | 0.43        | 0/304        |

| Mol | Chain | Bond lengths |                 | Bond angles |                 |
|-----|-------|--------------|-----------------|-------------|-----------------|
|     |       | RMSZ         | # Z  >5         | RMSZ        | # Z  >5         |
| 76  | AP    | 0.23         | 0/861           | 0.36        | 0/1136          |
| 77  | AQ    | 0.25         | 0/705           | 0.36        | 0/940           |
| 78  | AT    | 0.17         | 0/1813          | 0.31        | 0/2825          |
| 78  | PT    | 0.15         | 0/1813          | 0.27        | 0/2825          |
| 79  | MR    | 0.43         | 1/257 (0.4%)    | 0.32        | 0/397           |
| All | All   | 0.26         | 1/211469 (0.0%) | 0.37        | 3/310682 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 12  | C     | 0                   | 1                   |
| 27  | T     | 0                   | 1                   |
| 34  | Y     | 0                   | 1                   |
| All | All   | 0                   | 3                   |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 79  | MR    | 2   | U    | C1'-N1 | 5.83 | 1.57        | 1.48     |

All (3) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 42  | g     | 187 | HIS  | N-CA-C | 6.40  | 121.34      | 109.56   |
| 42  | g     | 186 | CYS  | CA-C-N | -5.24 | 114.96      | 122.67   |
| 42  | g     | 186 | CYS  | C-N-CA | -5.24 | 114.96      | 122.67   |

There are no chirality outliers.

All (3) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 12  | C     | 59  | ASP  | Peptide |
| 27  | T     | 102 | ALA  | Peptide |
| 34  | Y     | 88  | PRO  | 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     | 1442  | 0        | 1500     | 25      | 0            |
| 2   | 1     | 65536 | 0        | 32944    | 575     | 0            |
| 3   | 2     | 1276  | 0        | 1333     | 18      | 0            |
| 4   | 3     | 2579  | 0        | 1304     | 20      | 0            |
| 5   | 4     | 3313  | 0        | 1674     | 26      | 0            |
| 6   | 6     | 986   | 0        | 1040     | 16      | 0            |
| 7   | 7     | 516   | 0        | 534      | 11      | 0            |
| 8   | 8     | 960   | 0        | 1014     | 10      | 0            |
| 9   | 9     | 980   | 0        | 1058     | 9       | 0            |
| 10  | A     | 36083 | 0        | 18151    | 579     | 0            |
| 11  | B     | 1627  | 0        | 1644     | 58      | 0            |
| 12  | C     | 1724  | 0        | 1805     | 43      | 0            |
| 13  | D     | 1620  | 0        | 1715     | 34      | 0            |
| 14  | E     | 1701  | 0        | 1802     | 44      | 0            |
| 15  | F     | 2055  | 0        | 2137     | 36      | 0            |
| 16  | G     | 1572  | 0        | 1644     | 61      | 0            |
| 17  | H     | 1820  | 0        | 1896     | 49      | 0            |
| 18  | I     | 1466  | 0        | 1561     | 54      | 0            |
| 19  | J     | 1579  | 0        | 1602     | 32      | 0            |
| 20  | K     | 1453  | 0        | 1532     | 39      | 0            |
| 21  | L     | 783   | 0        | 799      | 32      | 0            |
| 22  | M     | 1129  | 0        | 1183     | 8       | 0            |
| 23  | N     | 539   | 0        | 573      | 22      | 0            |
| 24  | O     | 1187  | 0        | 1249     | 21      | 0            |
| 25  | P     | 942   | 0        | 980      | 29      | 0            |
| 26  | Q     | 906   | 0        | 940      | 36      | 0            |
| 27  | T     | 1169  | 0        | 1216     | 56      | 0            |
| 28  | R     | 1102  | 0        | 1168     | 61      | 0            |
| 29  | S     | 954   | 0        | 1008     | 36      | 0            |
| 30  | U     | 1100  | 0        | 1114     | 40      | 0            |
| 31  | V     | 790   | 0        | 855      | 24      | 0            |
| 32  | W     | 676   | 0        | 677      | 15      | 0            |
| 33  | X     | 1032  | 0        | 1066     | 20      | 0            |
| 34  | Y     | 1110  | 0        | 1182     | 15      | 0            |
| 35  | Z     | 1072  | 0        | 1123     | 32      | 0            |
| 36  | a     | 578   | 0        | 613      | 28      | 0            |
| 37  | b     | 779   | 0        | 832      | 19      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 38  | c     | 614   | 0        | 630      | 15      | 0            |
| 39  | d     | 487   | 0        | 523      | 24      | 0            |
| 40  | e     | 454   | 0        | 430      | 12      | 0            |
| 41  | f     | 461   | 0        | 499      | 11      | 0            |
| 42  | g     | 565   | 0        | 607      | 33      | 0            |
| 43  | h     | 1854  | 0        | 1793     | 83      | 0            |
| 44  | j     | 1894  | 0        | 1975     | 26      | 0            |
| 45  | k     | 3084  | 0        | 3173     | 40      | 0            |
| 46  | l     | 2751  | 0        | 2879     | 36      | 0            |
| 47  | m     | 2394  | 0        | 2362     | 29      | 0            |
| 48  | n     | 1237  | 0        | 1316     | 23      | 0            |
| 49  | o     | 1860  | 0        | 1958     | 18      | 0            |
| 50  | p     | 1795  | 0        | 1915     | 20      | 0            |
| 51  | q     | 1510  | 0        | 1582     | 16      | 0            |
| 52  | r     | 1759  | 0        | 1802     | 22      | 0            |
| 53  | s     | 1385  | 0        | 1418     | 34      | 0            |
| 54  | t     | 1573  | 0        | 1644     | 23      | 0            |
| 55  | u     | 1029  | 0        | 1116     | 14      | 0            |
| 56  | v     | 1713  | 0        | 1764     | 24      | 0            |
| 57  | w     | 1590  | 0        | 1705     | 16      | 0            |
| 58  | x     | 1375  | 0        | 1403     | 18      | 0            |
| 59  | y     | 1478  | 0        | 1590     | 20      | 0            |
| 60  | z     | 1471  | 0        | 1583     | 16      | 0            |
| 61  | AA    | 1087  | 0        | 1154     | 15      | 0            |
| 62  | AB    | 1170  | 0        | 1203     | 20      | 0            |
| 63  | AC    | 489   | 0        | 522      | 5       | 0            |
| 64  | AD    | 729   | 0        | 775      | 9       | 0            |
| 65  | AE    | 881   | 0        | 932      | 11      | 0            |
| 66  | AF    | 1015  | 0        | 1095     | 14      | 0            |
| 67  | AG    | 867   | 0        | 932      | 11      | 0            |
| 68  | AH    | 913   | 0        | 998      | 12      | 0            |
| 69  | AI    | 990   | 0        | 1094     | 14      | 0            |
| 70  | AJ    | 764   | 0        | 851      | 13      | 0            |
| 71  | AK    | 677   | 0        | 697      | 9       | 0            |
| 72  | AL    | 623   | 0        | 688      | 11      | 0            |
| 73  | AM    | 446   | 0        | 488      | 2       | 0            |
| 74  | AN    | 427   | 0        | 473      | 3       | 0            |
| 75  | AO    | 236   | 0        | 285      | 2       | 0            |
| 76  | AP    | 863   | 0        | 931      | 13      | 0            |
| 77  | AQ    | 698   | 0        | 734      | 6       | 0            |
| 78  | AT    | 1623  | 0        | 825      | 24      | 0            |
| 78  | PT    | 1623  | 0        | 825      | 19      | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 79  | MR    | 231    | 0        | 118      | 3       | 0            |
| 80  | 1     | 14     | 0        | 30       | 1       | 0            |
| 81  | 1     | 408    | 0        | 480      | 21      | 0            |
| 81  | A     | 136    | 0        | 160      | 7       | 0            |
| 81  | AT    | 34     | 0        | 40       | 1       | 0            |
| 82  | AH    | 1      | 0        | 0        | 0       | 0            |
| 82  | AK    | 1      | 0        | 0        | 0       | 0            |
| 82  | AN    | 1      | 0        | 0        | 0       | 0            |
| 82  | AP    | 1      | 0        | 0        | 0       | 0            |
| 82  | AQ    | 1      | 0        | 0        | 0       | 0            |
| 82  | b     | 1      | 0        | 0        | 0       | 0            |
| 82  | e     | 1      | 0        | 0        | 0       | 0            |
| All | All   | 197420 | 0        | 146465   | 2539    | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (2539) 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) |
|-------------------|------------------|--------------------------|-------------------|
| 2:1:2420:G:H1     | 2:1:2483:U:H3    | 1.01                     | 0.96              |
| 10:A:1341:U:H3    | 10:A:1352:G:H1   | 1.06                     | 0.93              |
| 10:A:478:G:H1     | 10:A:506:U:H3    | 1.15                     | 0.92              |
| 23:N:43:ARG:HH12  | 23:N:103:LEU:H   | 1.18                     | 0.90              |
| 2:1:2651:A:HO2'   | 53:s:52:TYR:HH   | 1.13                     | 0.89              |
| 78:AT:51:U:H3     | 78:AT:65:G:H1    | 0.91                     | 0.88              |
| 14:E:209:ILE:HD12 | 29:S:16:LEU:HD23 | 1.53                     | 0.88              |
| 10:A:1276:G:H1    | 10:A:1309:G:H22  | 1.16                     | 0.87              |
| 2:1:1560:U:H3     | 2:1:1571:G:H1    | 1.23                     | 0.86              |
| 10:A:1278:U:H3    | 10:A:1307:A:H62  | 1.24                     | 0.86              |
| 25:P:35:ALA:HB2   | 25:P:65:LYS:HG2  | 1.58                     | 0.85              |
| 2:1:2790:U:H5''   | 63:AC:1:MET:HA   | 1.57                     | 0.85              |
| 2:1:71:C:O2'      | 54:t:66:ASN:ND2  | 2.10                     | 0.84              |
| 46:l:111:ASN:HD22 | 56:v:201:ARG:HB3 | 1.40                     | 0.84              |
| 2:1:1756:A:N6     | 2:1:1762:G:C5    | 2.46                     | 0.84              |
| 2:1:3013:U:OP1    | 6:6:12:ARG:NH1   | 2.09                     | 0.83              |
| 2:1:1756:A:N6     | 2:1:1762:G:C6    | 2.47                     | 0.83              |
| 2:1:1436:G:OP1    | 46:l:84:HIS:NE2  | 2.12                     | 0.82              |
| 16:G:145:ASP:HB3  | 39:d:45:LYS:HE3  | 1.59                     | 0.82              |
| 10:A:1019:C:HO2'  | 33:X:2:THR:N     | 1.78                     | 0.82              |
| 10:A:869:A:O2'    | 12:C:124:ASN:ND2 | 2.13                     | 0.82              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 10:A:512:G:H1    | 10:A:541:C:H5     | 1.28                     | 0.81              |
| 28:R:12:LYS:HG3  | 28:R:13:LYS:H     | 1.43                     | 0.81              |
| 43:h:284:PRO:HB2 | 43:h:302:TYR:HB3  | 1.63                     | 0.80              |
| 2:1:1014:G:H22   | 2:1:1030:U:H3     | 1.28                     | 0.80              |
| 10:A:188:U:O2    | 10:A:193:G:N2     | 2.13                     | 0.80              |
| 11:B:23:HIS:HB3  | 11:B:50:ILE:HD11  | 1.61                     | 0.80              |
| 2:1:2380:A:H2'   | 46:l:68:THR:HG21  | 1.61                     | 0.80              |
| 10:A:1537:A:OP2  | 26:Q:42:ARG:NH2   | 2.16                     | 0.79              |
| 10:A:1324:C:O2'  | 10:A:1326:A:N7    | 2.15                     | 0.78              |
| 10:A:853:G:H1    | 10:A:945:U:H3     | 1.30                     | 0.78              |
| 20:K:127:VAL:O   | 20:K:131:GLN:NE2  | 2.17                     | 0.78              |
| 43:h:299:PHE:HB3 | 43:h:309:VAL:HA   | 1.66                     | 0.78              |
| 20:K:23:ARG:NH2  | 20:K:27:GLU:OE2   | 2.17                     | 0.78              |
| 16:G:83:ARG:NH2  | 16:G:86:GLN:OE1   | 2.16                     | 0.78              |
| 2:1:2334:A:H61   | 2:1:2955:C:H5     | 1.31                     | 0.78              |
| 43:h:122:GLN:N   | 43:h:122:GLN:HE21 | 1.82                     | 0.78              |
| 10:A:652:C:O2    | 10:A:678:A:N6     | 2.18                     | 0.77              |
| 27:T:84:TRP:HA   | 27:T:89:GLN:HE22  | 1.49                     | 0.77              |
| 65:AE:80:ASP:OD1 | 65:AE:81:GLU:N    | 2.16                     | 0.77              |
| 2:1:619:A:H2'    | 2:1:620:A:C8      | 2.20                     | 0.77              |
| 10:A:1575:G:H1   | 10:A:1595:U:H3    | 0.84                     | 0.77              |
| 2:1:1556:G:N7    | 8:8:36:LYS:NZ     | 2.31                     | 0.77              |
| 10:A:847:A:O2'   | 10:A:948:A:N1     | 2.18                     | 0.77              |
| 26:Q:58:LYS:HG2  | 26:Q:61:ARG:HH21  | 1.50                     | 0.76              |
| 51:q:8:GLN:HB3   | 51:q:72:LYS:HD3   | 1.67                     | 0.76              |
| 10:A:1156:A:H2'  | 10:A:1157:G:C8    | 2.21                     | 0.76              |
| 2:1:3139:U:OP2   | 67:AG:63:LYS:NZ   | 2.19                     | 0.76              |
| 13:D:30:TRP:O    | 13:D:41:LYS:NZ    | 2.18                     | 0.76              |
| 18:I:147:LYS:NZ  | 18:I:180:GLU:OE1  | 2.18                     | 0.76              |
| 47:m:182:GLY:HA2 | 47:m:194:LEU:HD23 | 1.66                     | 0.76              |
| 53:s:4:LYS:HG3   | 53:s:6:GLN:H      | 1.50                     | 0.76              |
| 10:A:803:G:H5'   | 10:A:804:U:H5'    | 1.68                     | 0.76              |
| 2:1:3192:A:O2'   | 55:u:126:LYS:NZ   | 2.19                     | 0.75              |
| 10:A:827:C:H3'   | 10:A:828:U:H5''   | 1.66                     | 0.75              |
| 2:1:2163:G:O2'   | 2:1:2292:U:OP2    | 2.02                     | 0.75              |
| 44:j:209:HIS:CE1 | 44:j:211:HIS:HD2  | 2.04                     | 0.75              |
| 61:AA:54:THR:H   | 61:AA:57:MET:HE2  | 1.51                     | 0.75              |
| 38:c:18:GLN:O    | 38:c:29:ARG:NH1   | 2.20                     | 0.75              |
| 16:G:48:PHE:HB2  | 16:G:67:PRO:HB3   | 1.68                     | 0.75              |
| 10:A:838:G:OP2   | 60:z:173:ARG:NH1  | 2.20                     | 0.75              |
| 5:4:66:A:OP1     | 69:AI:10:ARG:NH2  | 2.20                     | 0.75              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:H:116:GLN:NE2  | 17:H:119:ASN:O    | 2.19                     | 0.75              |
| 30:U:16:ASN:OD1   | 30:U:56:LYS:NZ    | 2.20                     | 0.74              |
| 2:1:1682:U:O2     | 2:1:1684:U:O2'    | 2.05                     | 0.74              |
| 26:Q:56:LEU:HD22  | 26:Q:80:LEU:HD21  | 1.70                     | 0.74              |
| 27:T:41:ARG:NH2   | 30:U:36:ILE:O     | 2.21                     | 0.74              |
| 17:H:14:LYS:HB3   | 17:H:124:LEU:HD11 | 1.66                     | 0.74              |
| 25:P:84:THR:HB    | 25:P:123:ARG:HG2  | 1.69                     | 0.74              |
| 2:1:3319:U:H3     | 19:J:107:THR:HG1  | 1.35                     | 0.74              |
| 10:A:78:A:H2      | 17:H:174:LYS:HG3  | 1.53                     | 0.74              |
| 10:A:1303:G:H5'   | 29:S:67:ARG:HH22  | 1.50                     | 0.74              |
| 16:G:55:ASP:OD2   | 16:G:57:SER:OG    | 2.04                     | 0.74              |
| 16:G:187:ILE:HD13 | 36:a:66:VAL:HG11  | 1.69                     | 0.74              |
| 36:a:59:TYR:HE1   | 36:a:100:ILE:HG23 | 1.53                     | 0.74              |
| 68:AH:38:ALA:O    | 68:AH:58:ARG:NH2  | 2.20                     | 0.74              |
| 52:r:36:LEU:HD21  | 52:r:69:ARG:HH11  | 1.53                     | 0.73              |
| 43:h:301:GLY:HA2  | 43:h:307:ILE:HA   | 1.69                     | 0.73              |
| 20:K:77:ILE:HD11  | 20:K:93:LEU:HD12  | 1.70                     | 0.73              |
| 53:s:49:LYS:NZ    | 76:AP:101:GLY:O   | 2.17                     | 0.73              |
| 2:1:437:G:H22     | 2:1:620:A:H61     | 1.36                     | 0.73              |
| 21:L:18:GLU:H     | 21:L:89:LEU:HB2   | 1.53                     | 0.73              |
| 45:k:35:ASP:OD2   | 45:k:191:LYS:NZ   | 2.21                     | 0.73              |
| 19:J:87:ASN:HB3   | 19:J:90:LEU:HD13  | 1.70                     | 0.73              |
| 11:B:93:THR:HB    | 11:B:185:ARG:HH22 | 1.52                     | 0.72              |
| 26:Q:81:ARG:NH2   | 26:Q:120:SER:O    | 2.21                     | 0.72              |
| 68:AH:58:ARG:HD3  | 68:AH:59:PRO:HD2  | 1.70                     | 0.72              |
| 23:N:35:SER:HA    | 23:N:38:HIS:HB2   | 1.70                     | 0.72              |
| 43:h:130:LYS:HG2  | 43:h:151:TRP:H    | 1.53                     | 0.72              |
| 10:A:1469:A:N3    | 10:A:1594:G:O2'   | 2.21                     | 0.72              |
| 30:U:130:ARG:HG2  | 30:U:134:ARG:HE   | 1.54                     | 0.72              |
| 10:A:835:A:H5'    | 60:z:165:ARG:HD3  | 1.69                     | 0.72              |
| 50:p:83:LEU:HD12  | 50:p:181:VAL:HG12 | 1.69                     | 0.72              |
| 46:l:139:ARG:HH21 | 46:l:241:PRO:HG2  | 1.55                     | 0.72              |
| 53:s:108:GLU:HG3  | 53:s:111:ASP:HB2  | 1.72                     | 0.72              |
| 2:1:538:G:H2'     | 2:1:539:G:C8      | 2.25                     | 0.71              |
| 44:j:209:HIS:HE1  | 44:j:211:HIS:HD2  | 1.35                     | 0.71              |
| 49:o:218:GLN:NE2  | 49:o:222:GLN:OE1  | 2.24                     | 0.71              |
| 54:t:63:VAL:HA    | 54:t:66:ASN:OD1   | 1.91                     | 0.71              |
| 69:AI:38:ARG:NH1  | 69:AI:40:SER:O    | 2.24                     | 0.71              |
| 27:T:88:ARG:NH2   | 27:T:91:ASP:OD1   | 2.23                     | 0.71              |
| 48:n:3:GLN:HG2    | 66:AF:76:LEU:H    | 1.54                     | 0.71              |
| 2:1:280:U:OP2     | 80:1:3401:SPK:N5  | 2.24                     | 0.71              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 13:D:51:ILE:HG23  | 13:D:56:LEU:HB2   | 1.72                     | 0.71              |
| 2:1:800:C:OP1     | 46:l:99:ARG:NH2   | 2.23                     | 0.71              |
| 16:G:62:ILE:HD11  | 16:G:89:ILE:HB    | 1.72                     | 0.71              |
| 2:1:564:G:H2'     | 2:1:565:A:C8      | 2.27                     | 0.70              |
| 10:A:1040:U:H3    | 10:A:1049:G:H1    | 1.38                     | 0.70              |
| 2:1:2420:G:N2     | 2:1:2483:U:O2     | 2.22                     | 0.70              |
| 14:E:29:GLU:OE2   | 21:L:56:LYS:NZ    | 2.24                     | 0.70              |
| 14:E:211:GLU:HA   | 29:S:19:ARG:HD3   | 1.73                     | 0.70              |
| 17:H:2:LYS:HB2    | 17:H:108:VAL:HG12 | 1.71                     | 0.70              |
| 15:F:191:ARG:HD2  | 15:F:246:LYS:HB2  | 1.74                     | 0.70              |
| 47:m:119:TYR:OH   | 47:m:139:PRO:O    | 2.08                     | 0.70              |
| 12:C:27:LYS:NZ    | 12:C:49:ASN:OD1   | 2.17                     | 0.69              |
| 35:Z:77:GLN:NE2   | 35:Z:81:ASP:OD2   | 2.19                     | 0.69              |
| 43:h:174:THR:HA   | 43:h:190:ILE:HG22 | 1.73                     | 0.69              |
| 15:F:35:PRO:HD2   | 15:F:83:PRO:HG2   | 1.74                     | 0.69              |
| 18:I:135:ARG:HB2  | 18:I:147:LYS:HB3  | 1.72                     | 0.69              |
| 30:U:29:GLU:H     | 30:U:110:LYS:HZ1  | 1.40                     | 0.69              |
| 53:s:26:SER:OG    | 53:s:64:LYS:O     | 2.10                     | 0.69              |
| 35:Z:74:LEU:HD12  | 35:Z:90:ARG:HH22  | 1.57                     | 0.69              |
| 46:l:299:VAL:HG21 | 59:y:132:PRO:HB2  | 1.74                     | 0.69              |
| 10:A:1024:A:O2'   | 10:A:1025:G:O5'   | 2.10                     | 0.69              |
| 12:C:190:PRO:O    | 12:C:195:ARG:NH2  | 2.26                     | 0.69              |
| 16:G:26:ALA:HB2   | 28:R:25:LYS:HG3   | 1.74                     | 0.69              |
| 18:I:95:LEU:O     | 18:I:108:ARG:NH1  | 2.26                     | 0.69              |
| 26:Q:100:LYS:HG3  | 26:Q:101:VAL:HG13 | 1.72                     | 0.69              |
| 2:1:1657:G:H2'    | 2:1:1658:G:C8     | 2.28                     | 0.69              |
| 18:I:149:LEU:HD12 | 18:I:182:PRO:HG3  | 1.75                     | 0.69              |
| 10:A:205:U:O2     | 19:J:184:ARG:NH1  | 2.24                     | 0.69              |
| 10:A:801:A:O4'    | 18:I:106:GLN:NE2  | 2.26                     | 0.69              |
| 62:AB:24:LYS:O    | 62:AB:26:ARG:HG2  | 1.93                     | 0.68              |
| 10:A:1742:A:O4'   | 34:Y:63:GLN:NE2   | 2.25                     | 0.68              |
| 1:0:130:GLU:HG2   | 1:0:131:LYS:HG3   | 1.73                     | 0.68              |
| 2:1:1949:G:H1     | 2:1:2070:A:H2'    | 1.58                     | 0.68              |
| 10:A:1784:A:H5'   | 37:b:95:ARG:HG2   | 1.75                     | 0.68              |
| 43:h:80:TYR:HD1   | 43:h:94:ASP:HA    | 1.58                     | 0.68              |
| 11:B:60:ALA:HA    | 11:B:63:ILE:HD12  | 1.75                     | 0.68              |
| 18:I:67:ARG:NH2   | 18:I:124:ASP:OD1  | 2.27                     | 0.68              |
| 2:1:62:A:OP1      | 56:v:172:ARG:NH2  | 2.27                     | 0.68              |
| 76:AP:38:GLN:OE1  | 76:AP:41:ARG:NH2  | 2.26                     | 0.68              |
| 10:A:592:A:OP1    | 20:K:40:ARG:NH2   | 2.24                     | 0.68              |
| 14:E:116:ILE:HD13 | 14:E:143:LEU:HD22 | 1.76                     | 0.68              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:G:53:VAL:HG13  | 16:G:138:VAL:HG11 | 1.76                     | 0.68              |
| 27:T:25:ARG:HG2   | 36:a:40:VAL:HG11  | 1.76                     | 0.68              |
| 10:A:1309:G:H4'   | 11:B:113:ARG:HH12 | 1.58                     | 0.68              |
| 2:1:1303:G:OP2    | 57:w:60:ARG:NH1   | 2.27                     | 0.68              |
| 14:E:73:LEU:HD23  | 21:L:20:VAL:HG13  | 1.76                     | 0.68              |
| 10:A:1275:U:H2'   | 10:A:1276:G:C8    | 2.28                     | 0.67              |
| 10:A:4:C:H5       | 10:A:20:G:H1      | 1.41                     | 0.67              |
| 10:A:821:U:H2'    | 10:A:822:G:H8     | 1.59                     | 0.67              |
| 10:A:1338:U:H2'   | 10:A:1339:G:H8    | 1.59                     | 0.67              |
| 22:M:26:LYS:HG2   | 22:M:27:ALA:H     | 1.58                     | 0.67              |
| 10:A:184:C:OP1    | 19:J:152:ARG:NH2  | 2.26                     | 0.67              |
| 10:A:1026:G:H2'   | 10:A:1027:G:C8    | 2.29                     | 0.67              |
| 10:A:1067:C:O2'   | 32:W:62:ARG:NH1   | 2.28                     | 0.67              |
| 52:r:53:VAL:HG21  | 52:r:166:ILE:HD12 | 1.77                     | 0.67              |
| 22:M:77:SER:HB3   | 22:M:85:ILE:HG12  | 1.76                     | 0.67              |
| 10:A:1485:G:H5'   | 30:U:72:GLY:HA3   | 1.77                     | 0.67              |
| 10:A:1597:G:H4'   | 16:G:98:MET:HE1   | 1.77                     | 0.67              |
| 27:T:29:MET:HB2   | 27:T:54:LEU:HD12  | 1.77                     | 0.67              |
| 29:S:60:ARG:HH22  | 29:S:66:VAL:HG21  | 1.59                     | 0.67              |
| 43:h:207:LEU:HD12 | 43:h:219:LEU:HD21 | 1.74                     | 0.67              |
| 16:G:133:VAL:HG22 | 16:G:198:LEU:HD13 | 1.77                     | 0.67              |
| 51:q:105:LYS:NZ   | 51:q:110:ASP:OD1  | 2.27                     | 0.67              |
| 70:AJ:56:LEU:HD22 | 70:AJ:89:MET:HG3  | 1.76                     | 0.67              |
| 2:1:2740:U:H2'    | 2:1:2741:A:H8     | 1.60                     | 0.67              |
| 15:F:31:PRO:HG2   | 15:F:38:LEU:HG    | 1.76                     | 0.67              |
| 18:I:172:LEU:HD12 | 18:I:173:THR:HG23 | 1.77                     | 0.67              |
| 39:d:11:LYS:HA    | 39:d:53:ILE:HA    | 1.77                     | 0.67              |
| 10:A:1037:U:O2    | 10:A:1052:G:N2    | 2.28                     | 0.67              |
| 16:G:143:ARG:N    | 16:G:218:GLU:OE2  | 2.28                     | 0.66              |
| 35:Z:56:SER:HB3   | 35:Z:74:LEU:HB2   | 1.75                     | 0.66              |
| 10:A:444:A:H5''   | 15:F:57:ASN:HD22  | 1.59                     | 0.66              |
| 10:A:691:U:H5'    | 10:A:692:U:H5''   | 1.77                     | 0.66              |
| 2:1:438:A:N1      | 2:1:489:G:O2'     | 2.21                     | 0.66              |
| 72:AL:40:GLN:HE21 | 72:AL:55:VAL:HG13 | 1.60                     | 0.66              |
| 2:1:2191:A:H2'    | 2:1:2192:A:C8     | 2.30                     | 0.66              |
| 29:S:41:ILE:HG22  | 29:S:43:SER:H     | 1.61                     | 0.66              |
| 2:1:1936:G:H21    | 2:1:3327:A:H8     | 1.42                     | 0.66              |
| 2:1:2808:OMC:H5   | 2:1:2824:C:H42    | 1.43                     | 0.66              |
| 18:I:40:LYS:HE3   | 18:I:59:PRO:HG3   | 1.77                     | 0.66              |
| 48:n:71:ASN:ND2   | 48:n:159:LEU:O    | 2.22                     | 0.66              |
| 2:1:1345:G:N2     | 46:l:292:ASN:O    | 2.29                     | 0.66              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:1:3278:U:H4'    | 45:k:173:GLN:HG3   | 1.78                     | 0.66              |
| 10:A:1300:U:HO2'  | 10:A:1301:G:H8     | 1.43                     | 0.66              |
| 10:A:1579:A:H2'   | 10:A:1580:A:H8     | 1.60                     | 0.66              |
| 11:B:189:PRO:HD2  | 11:B:193:THR:HG21  | 1.77                     | 0.66              |
| 30:U:42:GLY:HA3   | 30:U:94:VAL:HG21   | 1.77                     | 0.66              |
| 26:Q:56:LEU:HD13  | 26:Q:78:THR:HG21   | 1.77                     | 0.66              |
| 45:k:108:GLU:OE1  | 45:k:109:HIS:NE2   | 2.28                     | 0.66              |
| 49:o:108:GLN:HE22 | 49:o:204:LYS:HG2   | 1.59                     | 0.66              |
| 11:B:112:THR:HG22 | 11:B:114:SER:H     | 1.60                     | 0.66              |
| 16:G:34:GLN:HA    | 16:G:37:GLN:HE22   | 1.61                     | 0.66              |
| 29:S:23:LYS:HB3   | 29:S:34:LEU:HD11   | 1.76                     | 0.66              |
| 2:1:1091:U:H4'    | 2:1:1092:U:H5'     | 1.77                     | 0.66              |
| 10:A:856:G:H2'    | 10:A:857:G:C8      | 2.30                     | 0.66              |
| 27:T:25:ARG:NH2   | 36:a:38:HIS:O      | 2.29                     | 0.66              |
| 30:U:66:TYR:HD1   | 30:U:67:LEU:HD22   | 1.61                     | 0.66              |
| 43:h:44:LYS:HZ3   | 43:h:95:LEU:HB3    | 1.59                     | 0.66              |
| 61:AA:111:LYS:HA  | 61:AA:114:VAL:HG12 | 1.76                     | 0.66              |
| 10:A:45:U:O2'     | 10:A:46:A:H2'      | 1.96                     | 0.65              |
| 27:T:70:VAL:O     | 27:T:74:GLN:NE2    | 2.29                     | 0.65              |
| 2:1:339:C:OP1     | 2:1:1376:G:O2'     | 2.14                     | 0.65              |
| 14:E:95:ARG:HB3   | 14:E:101:VAL:HG11  | 1.77                     | 0.65              |
| 10:A:1156:A:H2'   | 10:A:1157:G:H8     | 1.59                     | 0.65              |
| 10:A:1459:U:O4    | 16:G:180:ARG:NH1   | 2.29                     | 0.65              |
| 10:A:1578:C:H2'   | 10:A:1579:A:H8     | 1.62                     | 0.65              |
| 27:T:88:ARG:HD3   | 27:T:108:LYS:HE2   | 1.78                     | 0.65              |
| 28:R:82:GLN:HE22  | 28:R:86:LYS:HD2    | 1.62                     | 0.65              |
| 10:A:62:A:H8      | 10:A:285:G:H21     | 1.42                     | 0.65              |
| 23:N:43:ARG:NH1   | 23:N:101:ALA:O     | 2.28                     | 0.65              |
| 6:6:13:MET:HE1    | 6:6:54:ALA:HB3     | 1.78                     | 0.65              |
| 10:A:330:U:OP1    | 19:J:56:ARG:NH2    | 2.29                     | 0.65              |
| 25:P:15:PHE:HB3   | 25:P:22:PHE:HB2    | 1.79                     | 0.65              |
| 43:h:174:THR:HG23 | 43:h:176:LYS:HG3   | 1.78                     | 0.65              |
| 54:t:124:VAL:HG21 | 69:AI:120:ALA:HB3  | 1.78                     | 0.65              |
| 10:A:64:U:O2'     | 10:A:166:A:N3      | 2.28                     | 0.65              |
| 10:A:1226:G:H5''  | 26:Q:77:LYS:HG3    | 1.78                     | 0.65              |
| 18:I:5:ILE:HG22   | 18:I:7:SER:H       | 1.62                     | 0.65              |
| 11:B:198:MET:HE1  | 11:B:200:ASP:HB2   | 1.79                     | 0.65              |
| 28:R:45:PHE:HA    | 28:R:48:TYR:HB2    | 1.79                     | 0.65              |
| 10:A:932:U:OP1    | 12:C:165:ARG:NH1   | 2.29                     | 0.65              |
| 15:F:199:GLU:OE2  | 15:F:201:HIS:NE2   | 2.25                     | 0.65              |
| 16:G:100:ASN:HB2  | 16:G:180:ARG:HD3   | 1.79                     | 0.65              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 28:R:6:VAL:HG12   | 28:R:94:LYS:HD3    | 1.78                     | 0.65              |
| 30:U:14:PHE:HE1   | 30:U:136:ALA:HB2   | 1.62                     | 0.65              |
| 10:A:838:G:OP2    | 60:z:176:ARG:NH2   | 2.30                     | 0.64              |
| 43:h:203:PRO:HG3  | 43:h:244:PRO:HA    | 1.78                     | 0.64              |
| 20:K:87:SER:OG    | 20:K:89:ASP:OD1    | 2.15                     | 0.64              |
| 25:P:21:THR:HG21  | 25:P:55:ALA:HB2    | 1.78                     | 0.64              |
| 55:u:120:ARG:NH1  | 57:w:186:THR:O     | 2.30                     | 0.64              |
| 27:T:53:GLU:HG2   | 27:T:55:THR:HG22   | 1.79                     | 0.64              |
| 30:U:4:VAL:HG21   | 30:U:140:LEU:HG    | 1.80                     | 0.64              |
| 53:s:109:HIS:HB2  | 53:s:114:ILE:HD12  | 1.78                     | 0.64              |
| 2:1:976:A:N6      | 2:1:1100:G:O2'     | 2.31                     | 0.64              |
| 14:E:173:ILE:HG12 | 14:E:186:LYS:HG2   | 1.78                     | 0.64              |
| 48:n:39:LEU:HD13  | 48:n:83:VAL:HG11   | 1.79                     | 0.64              |
| 2:1:3039:C:H3'    | 60:z:62:ARG:HH22   | 1.62                     | 0.64              |
| 51:q:47:LYS:HB2   | 55:u:5:VAL:HG22    | 1.80                     | 0.64              |
| 2:1:591:C:O2      | 49:o:24:ARG:NH1    | 2.31                     | 0.64              |
| 2:1:226:G:H5'     | 81:1:3410:GET:H831 | 1.79                     | 0.64              |
| 2:1:266:C:OP1     | 56:v:5:LYS:NZ      | 2.28                     | 0.64              |
| 10:A:1204:A:H62   | 10:A:1249:G:H21    | 1.46                     | 0.64              |
| 65:AE:45:THR:HG22 | 65:AE:47:ASP:H     | 1.63                     | 0.64              |
| 10:A:636:C:O2'    | 18:I:97:LYS:NZ     | 2.30                     | 0.64              |
| 10:A:1222:G:N1    | 10:A:1234:U:O4     | 2.30                     | 0.64              |
| 10:A:1168:A:N3    | 10:A:1195:C:O2'    | 2.27                     | 0.63              |
| 57:w:122:PRO:HA   | 57:w:125:LEU:HD12  | 1.79                     | 0.63              |
| 2:1:1720:U:H1'    | 2:1:1721:C:C6      | 2.33                     | 0.63              |
| 10:A:1458:C:H41   | 10:A:1523:G:H1     | 1.47                     | 0.63              |
| 27:T:102:ALA:O    | 27:T:104:ASN:N     | 2.31                     | 0.63              |
| 61:AA:53:VAL:HG11 | 61:AA:62:VAL:HG13  | 1.81                     | 0.63              |
| 21:L:12:HIS:HB3   | 21:L:80:LEU:HD11   | 1.80                     | 0.63              |
| 25:P:87:LYS:NZ    | 25:P:115:PRO:O     | 2.32                     | 0.63              |
| 10:A:405:A:H2'    | 10:A:406:C:C6      | 2.34                     | 0.63              |
| 1:0:52:LYS:NZ     | 4:3:101:G:N7       | 2.40                     | 0.63              |
| 39:d:10:ALA:HB1   | 39:d:30:VAL:HB     | 1.80                     | 0.63              |
| 43:h:22:SER:HB3   | 43:h:36:GLY:HA3    | 1.78                     | 0.63              |
| 45:k:313:ARG:O    | 45:k:333:LYS:NZ    | 2.28                     | 0.63              |
| 56:v:33:LYS:O     | 56:v:65:ARG:NH2    | 2.32                     | 0.63              |
| 2:1:1491:U:H5     | 2:1:1831:A:N1      | 1.97                     | 0.63              |
| 10:A:883:A:H61    | 10:A:899:G:H1'     | 1.62                     | 0.63              |
| 31:V:32:GLN:NE2   | 31:V:109:PRO:O     | 2.31                     | 0.63              |
| 52:r:207:GLU:OE2  | 52:r:211:GLN:NE2   | 2.31                     | 0.63              |
| 10:A:1584:A:C8    | 40:e:14:PHE:HB2    | 2.33                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:T:17:LEU:HG    | 27:T:18:LEU:H     | 1.64                     | 0.63              |
| 45:k:372:THR:HG22 | 45:k:374:ALA:H    | 1.62                     | 0.63              |
| 1:0:82:GLU:HG2    | 1:0:87:ILE:HG12   | 1.81                     | 0.63              |
| 18:I:121:ILE:HG21 | 18:I:172:LEU:HD11 | 1.80                     | 0.63              |
| 26:Q:94:VAL:HG11  | 26:Q:116:LEU:HD11 | 1.80                     | 0.63              |
| 36:a:65:LEU:HB3   | 36:a:69:LEU:HD12  | 1.81                     | 0.63              |
| 43:h:113:SER:HB2  | 43:h:154:ALA:HA   | 1.81                     | 0.63              |
| 10:A:1276:G:H22   | 10:A:1309:G:N2    | 1.95                     | 0.62              |
| 12:C:90:GLU:OE2   | 12:C:92:GLN:NE2   | 2.32                     | 0.62              |
| 76:AP:8:ARG:NH1   | 76:AP:10:THR:HG21 | 2.14                     | 0.62              |
| 10:A:1342:A:H2'   | 10:A:1343:G:H8    | 1.65                     | 0.62              |
| 27:T:16:ARG:NH1   | 27:T:17:LEU:O     | 2.31                     | 0.62              |
| 2:1:2504:C:OP1    | 44:j:37:ARG:NH2   | 2.29                     | 0.62              |
| 2:1:2932:C:H2'    | 2:1:2933:G:C8     | 2.34                     | 0.62              |
| 10:A:126:A:H62    | 10:A:289:G:H21    | 1.46                     | 0.62              |
| 10:A:261:C:O2'    | 10:A:262:G:N2     | 2.25                     | 0.62              |
| 10:A:530:U:OP1    | 35:Z:64:PHE:HA    | 1.99                     | 0.62              |
| 39:d:31:GLU:HG2   | 39:d:32:PHE:H     | 1.64                     | 0.62              |
| 44:j:101:ILE:HG13 | 44:j:165:VAL:HG22 | 1.82                     | 0.62              |
| 10:A:821:U:H2'    | 10:A:822:G:C8     | 2.34                     | 0.62              |
| 21:L:81:ASN:HB2   | 23:N:37:VAL:HG21  | 1.81                     | 0.62              |
| 23:N:43:ARG:HG2   | 23:N:121:VAL:HB   | 1.81                     | 0.62              |
| 10:A:65:A:OP1     | 17:H:176:GLN:NE2  | 2.31                     | 0.62              |
| 10:A:193:G:N7     | 19:J:147:ARG:NH2  | 2.47                     | 0.62              |
| 10:A:1578:C:H2'   | 10:A:1579:A:C8    | 2.35                     | 0.62              |
| 14:E:40:VAL:HG12  | 14:E:49:VAL:HG22  | 1.82                     | 0.62              |
| 37:b:23:CYS:HB3   | 37:b:28:ARG:H     | 1.65                     | 0.62              |
| 1:0:155:ARG:HD3   | 1:0:172:TYR:CD1   | 2.34                     | 0.62              |
| 10:A:1579:A:H2'   | 10:A:1580:A:C8    | 2.34                     | 0.62              |
| 27:T:68:ARG:O     | 27:T:72:ILE:HG13  | 1.99                     | 0.62              |
| 42:g:182:TYR:OH   | 42:g:187:HIS:ND1  | 2.28                     | 0.62              |
| 45:k:95:THR:OG1   | 45:k:98:GLY:O     | 2.15                     | 0.62              |
| 65:AE:76:ARG:HD3  | 65:AE:88:LEU:HD13 | 1.82                     | 0.62              |
| 12:C:59:ASP:OD1   | 12:C:60:GLY:N     | 2.32                     | 0.62              |
| 22:M:16:GLN:HB3   | 22:M:19:ILE:HD13  | 1.82                     | 0.62              |
| 24:O:91:LEU:HB3   | 24:O:122:ILE:HG12 | 1.82                     | 0.62              |
| 10:A:511:U:H2'    | 10:A:512:G:C8     | 2.35                     | 0.62              |
| 14:E:107:LYS:HG3  | 14:E:176:VAL:HG22 | 1.81                     | 0.62              |
| 26:Q:75:VAL:HA    | 26:Q:93:VAL:HG13  | 1.82                     | 0.62              |
| 28:R:93:GLN:NE2   | 43:h:61:SER:O     | 2.33                     | 0.62              |
| 47:m:60:ILE:HB    | 47:m:80:ALA:HB2   | 1.82                     | 0.62              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 78:AT:4:G:H1      | 78:AT:70:C:H42     | 1.48                     | 0.62              |
| 43:h:70:GLN:OE1   | 43:h:86:TRP:NE1    | 2.26                     | 0.61              |
| 10:A:1672:G:H2'   | 10:A:1674:U:C4     | 2.35                     | 0.61              |
| 14:E:46:LYS:HE3   | 14:E:86:ALA:HB2    | 1.82                     | 0.61              |
| 18:I:34:LEU:HD21  | 18:I:73:LEU:HD21   | 1.81                     | 0.61              |
| 23:N:45:LEU:HD11  | 42:g:142:LEU:HG    | 1.82                     | 0.61              |
| 2:1:511:C:OP1     | 46:l:344:LYS:NZ    | 2.24                     | 0.61              |
| 2:1:2210:A:H2'    | 2:1:2211:A:C8      | 2.36                     | 0.61              |
| 81:A:1804:GET:N32 | 79:MR:11:U:OP1     | 2.32                     | 0.61              |
| 11:B:172:LEU:O    | 11:B:176:LEU:HG    | 2.00                     | 0.61              |
| 21:L:70:ASP:OD1   | 21:L:91:ARG:NH2    | 2.34                     | 0.61              |
| 2:1:1091:U:O4'    | 3:2:129:LYS:NZ     | 2.33                     | 0.61              |
| 15:F:50:ASN:O     | 15:F:53:LYS:NZ     | 2.32                     | 0.61              |
| 16:G:41:LYS:HB2   | 16:G:44:ASN:HA     | 1.80                     | 0.61              |
| 22:M:27:ALA:HA    | 22:M:29:LYS:HE3    | 1.82                     | 0.61              |
| 10:A:920:U:O4     | 37:b:15:ARG:NH1    | 2.33                     | 0.61              |
| 17:H:77:LEU:HD12  | 17:H:95:LYS:HD3    | 1.82                     | 0.61              |
| 31:V:52:LYS:HB3   | 31:V:91:ASP:HB2    | 1.83                     | 0.61              |
| 28:R:68:VAL:HG11  | 28:R:80:ILE:HD11   | 1.81                     | 0.61              |
| 50:p:63:LYS:NZ    | 56:v:29:GLU:OE1    | 2.30                     | 0.61              |
| 2:1:732:U:H3'     | 2:1:733:A:H8       | 1.65                     | 0.61              |
| 2:1:1099:A:N6     | 2:1:1359:A:H1'     | 2.15                     | 0.61              |
| 2:1:3287:A:H2'    | 2:1:3288:A:C8      | 2.34                     | 0.61              |
| 27:T:56:LYS:HB2   | 27:T:60:GLU:HG3    | 1.82                     | 0.61              |
| 31:V:36:VAL:HG11  | 31:V:111:VAL:HG11  | 1.83                     | 0.61              |
| 46:l:301:ARG:NH1  | 59:y:38:ARG:O      | 2.33                     | 0.61              |
| 77:AQ:88:GLU:HA   | 77:AQ:91:GLU:HG2   | 1.82                     | 0.61              |
| 2:1:437:G:N2      | 2:1:620:A:H61      | 1.99                     | 0.61              |
| 10:A:917:U:OP2    | 12:C:155:TYR:OH    | 2.14                     | 0.61              |
| 13:D:32:PRO:HB2   | 13:D:38:ARG:HG3    | 1.82                     | 0.61              |
| 38:c:56:CYS:HB2   | 38:c:63:LEU:HD21   | 1.83                     | 0.61              |
| 10:A:1463:G:H2'   | 10:A:1464:G:C8     | 2.35                     | 0.61              |
| 12:C:25:THR:O     | 12:C:50:ARG:NH2    | 2.33                     | 0.61              |
| 18:I:11:THR:HG22  | 18:I:14:GLU:HG2    | 1.83                     | 0.61              |
| 18:I:66:TYR:O     | 18:I:70:GLN:HB2    | 2.01                     | 0.61              |
| 66:AF:112:LYS:HE2 | 66:AF:116:LEU:HD11 | 1.82                     | 0.61              |
| 10:A:1242:U:H2'   | 21:L:2:LEU:HA      | 1.82                     | 0.60              |
| 10:A:1559:G:O2'   | 16:G:185:ARG:NH2   | 2.34                     | 0.60              |
| 30:U:27:LYS:HE2   | 30:U:111:ILE:HG23  | 1.83                     | 0.60              |
| 43:h:133:LYS:HE2  | 43:h:141:CYS:SG    | 2.41                     | 0.60              |
| 69:AI:92:LEU:HD22 | 69:AI:96:GLU:HB3   | 1.81                     | 0.60              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:1:2244:U:OP1   | 78:PT:25:U:O2'    | 2.20                     | 0.60              |
| 28:R:21:VAL:HG13 | 28:R:64:ILE:HG22  | 1.83                     | 0.60              |
| 58:x:169:ASN:OD1 | 67:AG:60:ARG:NH1  | 2.33                     | 0.60              |
| 62:AB:60:TYR:CE2 | 62:AB:63:LYS:HA   | 2.36                     | 0.60              |
| 10:A:482:C:H3'   | 10:A:483:A:H5''   | 1.82                     | 0.60              |
| 10:A:1474:G:O2'  | 10:A:1481:C:O2    | 2.18                     | 0.60              |
| 2:1:1949:G:N2    | 2:1:2070:A:O2'    | 2.33                     | 0.60              |
| 10:A:1183:G:OP1  | 10:A:1184:G:O2'   | 2.13                     | 0.60              |
| 10:A:1420:U:H4'  | 40:e:24:CYS:HB2   | 1.83                     | 0.60              |
| 37:b:40:THR:OG1  | 37:b:69:ASN:OD1   | 2.20                     | 0.60              |
| 43:h:64:GLY:O    | 43:h:91:ARG:NH1   | 2.30                     | 0.60              |
| 50:p:28:PHE:HE1  | 61:AA:53:VAL:HG12 | 1.65                     | 0.60              |
| 10:A:1395:G:N2   | 10:A:1398:G:OP2   | 2.32                     | 0.60              |
| 10:A:1460:G:H2'  | 10:A:1461:A:H8    | 1.66                     | 0.60              |
| 10:A:1668:A:H1'  | 17:H:66:GLY:HA2   | 1.83                     | 0.60              |
| 29:S:74:GLN:HB3  | 29:S:78:ARG:HE    | 1.66                     | 0.60              |
| 31:V:60:LYS:HB2  | 31:V:85:ILE:HB    | 1.84                     | 0.60              |
| 10:A:915:A:N3    | 12:C:111:ARG:NH2  | 2.49                     | 0.60              |
| 10:A:1145:A:H2'  | 10:A:1146:C:C6    | 2.36                     | 0.60              |
| 13:D:147:HIS:ND1 | 13:D:190:ASP:OD2  | 2.34                     | 0.60              |
| 26:Q:56:LEU:HA   | 26:Q:59:LYS:HE2   | 1.83                     | 0.60              |
| 10:A:1567:C:H4'  | 28:R:136:ARG:HB2  | 1.84                     | 0.60              |
| 38:c:42:ASN:C    | 38:c:42:ASN:HD22  | 2.09                     | 0.60              |
| 2:1:1099:A:H61   | 2:1:1359:A:H1'    | 1.66                     | 0.60              |
| 2:1:3208:A:H4'   | 45:k:95:THR:HG22  | 1.84                     | 0.60              |
| 10:A:589:A:H2'   | 10:A:590:A:C8     | 2.36                     | 0.60              |
| 11:B:84:ARG:HD3  | 11:B:204:TYR:HA   | 1.84                     | 0.60              |
| 2:1:1611:U:H2'   | 2:1:1612:U:C6     | 2.35                     | 0.60              |
| 29:S:7:LYS:HD2   | 29:S:11:ARG:HH21  | 1.65                     | 0.60              |
| 10:A:1630:U:OP1  | 81:A:1802:GET:N21 | 2.35                     | 0.60              |
| 28:R:98:GLU:OE2  | 43:h:58:PRO:HB2   | 2.02                     | 0.60              |
| 2:1:1012:U:O2'   | 2:1:1013:U:O5'    | 2.20                     | 0.59              |
| 10:A:627:U:OP1   | 24:O:127:ARG:NH2  | 2.35                     | 0.59              |
| 12:C:151:LYS:NZ  | 12:C:153:THR:O    | 2.30                     | 0.59              |
| 51:q:57:VAL:HG23 | 51:q:68:LEU:HD13  | 1.82                     | 0.59              |
| 1:0:71:LYS:NZ    | 2:1:561:U:OP1     | 2.35                     | 0.59              |
| 2:1:437:G:H22    | 2:1:620:A:N6      | 2.00                     | 0.59              |
| 10:A:764:U:C2    | 35:Z:8:ARG:HD3    | 2.37                     | 0.59              |
| 18:I:94:ILE:HG12 | 18:I:117:VAL:HG21 | 1.84                     | 0.59              |
| 2:1:1115:C:H2'   | 2:1:1116:A:H8     | 1.68                     | 0.59              |
| 10:A:1342:A:H2'  | 10:A:1343:G:C8    | 2.37                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:1:2740:U:H2'    | 2:1:2741:A:C8     | 2.38                     | 0.59              |
| 6:6:135:VAL:HG11  | 7:7:26:SER:HB3    | 1.84                     | 0.59              |
| 26:Q:21:ASP:OD1   | 26:Q:22:LEU:N     | 2.34                     | 0.59              |
| 43:h:253:THR:OG1  | 43:h:256:GLY:O    | 2.14                     | 0.59              |
| 2:1:2285:G:O2'    | 2:1:2288:U:OP2    | 2.17                     | 0.59              |
| 18:I:95:LEU:HB2   | 18:I:112:ARG:HB3  | 1.84                     | 0.59              |
| 2:1:3308:G:H21    | 2:1:3327:A:H2     | 1.47                     | 0.59              |
| 9:9:52:GLN:O      | 9:9:70:VAL:HB     | 2.03                     | 0.59              |
| 21:L:15:LEU:O     | 21:L:19:GLY:HA2   | 2.03                     | 0.59              |
| 29:S:17:ILE:HG12  | 29:S:58:MET:HE2   | 1.85                     | 0.59              |
| 44:j:211:HIS:ND1  | 44:j:219:ILE:HG23 | 2.18                     | 0.59              |
| 1:0:168:PRO:HG3   | 57:w:125:LEU:HD13 | 1.84                     | 0.59              |
| 10:A:1554:U:H4'   | 27:T:36:ARG:HE    | 1.67                     | 0.59              |
| 10:A:1575:G:O6    | 10:A:1595:U:O4    | 2.20                     | 0.59              |
| 30:U:5:SER:OG     | 30:U:6:VAL:N      | 2.33                     | 0.59              |
| 2:1:654:A:H2'     | 2:1:655:A:C8      | 2.38                     | 0.59              |
| 10:A:188:U:H3     | 10:A:193:G:H1     | 1.51                     | 0.59              |
| 10:A:945:U:H5'    | 24:O:55:ARG:HD3   | 1.85                     | 0.59              |
| 14:E:43:THR:OG1   | 14:E:46:LYS:O     | 2.21                     | 0.59              |
| 2:1:93:G:H2'      | 2:1:94:A:C8       | 2.38                     | 0.59              |
| 2:1:2506:G:H5''   | 50:p:249:LYS:HE3  | 1.85                     | 0.59              |
| 10:A:1546:G:H5''  | 27:T:135:GLY:HA3  | 1.85                     | 0.59              |
| 13:D:218:SER:HB3  | 32:W:25:LYS:HD3   | 1.83                     | 0.59              |
| 24:O:17:PRO:HG3   | 38:c:28:PRO:HG3   | 1.85                     | 0.59              |
| 52:r:30:LYS:HG3   | 52:r:63:GLU:HG3   | 1.83                     | 0.59              |
| 10:A:811:U:H2'    | 10:A:812:C:H6     | 1.68                     | 0.58              |
| 10:A:1041:C:N3    | 10:A:1048:U:O4    | 2.36                     | 0.58              |
| 2:1:896:G:H1'     | 2:1:1585:A:N6     | 2.18                     | 0.58              |
| 2:1:3260:A:H2'    | 2:1:3261:A:C8     | 2.38                     | 0.58              |
| 10:A:883:A:N6     | 10:A:899:G:H1'    | 2.17                     | 0.58              |
| 11:B:180:GLU:CD   | 11:B:191:ARG:HH12 | 2.10                     | 0.58              |
| 15:F:105:VAL:HG23 | 15:F:191:ARG:HG2  | 1.85                     | 0.58              |
| 20:K:148:VAL:HG11 | 20:K:156:ILE:HD11 | 1.85                     | 0.58              |
| 30:U:40:SER:HB3   | 30:U:43:ASN:HB2   | 1.85                     | 0.58              |
| 42:g:162:GLU:OE1  | 42:g:171:GLY:N    | 2.35                     | 0.58              |
| 2:1:1344:U:OP1    | 59:y:39:ARG:NH1   | 2.36                     | 0.58              |
| 4:3:112:G:H2'     | 4:3:113:C:C6      | 2.39                     | 0.58              |
| 10:A:151:G:H2'    | 10:A:152:G:C8     | 2.38                     | 0.58              |
| 10:A:811:U:H2'    | 10:A:812:C:C6     | 2.38                     | 0.58              |
| 10:A:1526:G:H4'   | 27:T:40:ARG:HH22  | 1.66                     | 0.58              |
| 18:I:31:LYS:HD3   | 18:I:35:ARG:HH21  | 1.67                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 24:O:4:MET:HG2    | 24:O:5:HIS:CD2    | 2.39                     | 0.58              |
| 50:p:92:PHE:O     | 50:p:96:ASN:ND2   | 2.36                     | 0.58              |
| 2:1:2653:U:H5'    | 53:s:65:ILE:HD11  | 1.86                     | 0.58              |
| 10:A:478:G:N2     | 10:A:506:U:O2     | 2.32                     | 0.58              |
| 10:A:892:A:H2'    | 10:A:893:U:H6     | 1.67                     | 0.58              |
| 36:a:78:VAL:HA    | 36:a:81:ARG:HD2   | 1.84                     | 0.58              |
| 45:k:58:ARG:HD2   | 45:k:354:VAL:HB   | 1.85                     | 0.58              |
| 2:1:653:C:H2'     | 2:1:654:A:C8      | 2.38                     | 0.58              |
| 2:1:827:G:O2'     | 2:1:1860:A:N3     | 2.34                     | 0.58              |
| 10:A:697:U:H3     | 10:A:724:G:H1     | 1.52                     | 0.58              |
| 10:A:1520:C:OP1   | 27:T:27:LYS:NZ    | 2.25                     | 0.58              |
| 2:1:25:A:N3       | 2:1:328:U:O2'     | 2.36                     | 0.58              |
| 2:1:2941:A:N7     | 44:j:215:ASN:ND2  | 2.52                     | 0.58              |
| 10:A:219:A:N1     | 10:A:827:C:N4     | 2.52                     | 0.58              |
| 10:A:516:A:H2'    | 10:A:517:C:H5''   | 1.86                     | 0.58              |
| 50:p:160:PRO:HB2  | 50:p:162:GLU:OE1  | 2.04                     | 0.58              |
| 29:S:12:ALA:O     | 29:S:16:LEU:HG    | 2.04                     | 0.58              |
| 36:a:65:LEU:O     | 36:a:69:LEU:HB2   | 2.03                     | 0.58              |
| 53:s:59:ILE:HD11  | 53:s:65:ILE:HD13  | 1.85                     | 0.58              |
| 10:A:1676:A:H1'   | 10:A:1701:A:C2    | 2.39                     | 0.58              |
| 30:U:84:LYS:HE2   | 30:U:94:VAL:HG11  | 1.86                     | 0.58              |
| 2:1:1713:U:H2'    | 2:1:1714:G:C8     | 2.39                     | 0.57              |
| 10:A:635:C:O2     | 18:I:110:ARG:NH1  | 2.37                     | 0.57              |
| 12:C:62:LYS:HE3   | 12:C:89:ASP:C     | 2.28                     | 0.57              |
| 12:C:195:ARG:O    | 12:C:199:LYS:HG2  | 2.04                     | 0.57              |
| 41:f:4:VAL:HG11   | 78:AT:37:U:H4'    | 1.85                     | 0.57              |
| 43:h:90:LEU:HB2   | 43:h:104:PHE:HB2  | 1.85                     | 0.57              |
| 17:H:195:VAL:O    | 17:H:199:GLN:HG2  | 2.04                     | 0.57              |
| 35:Z:57:VAL:HB    | 35:Z:60:PHE:HE2   | 1.67                     | 0.57              |
| 46:l:351:LYS:O    | 46:l:354:LYS:NZ   | 2.28                     | 0.57              |
| 2:1:660:U:H2'     | 2:1:661:C:C6      | 2.39                     | 0.57              |
| 13:D:47:SER:OG    | 13:D:49:GLU:OE1   | 2.23                     | 0.57              |
| 16:G:111:VAL:HA   | 16:G:114:VAL:HG22 | 1.85                     | 0.57              |
| 21:L:32:HIS:HD2   | 21:L:35:ILE:HB    | 1.70                     | 0.57              |
| 44:j:111:THR:HB   | 44:j:136:ILE:HD12 | 1.85                     | 0.57              |
| 67:AG:49:ILE:HD11 | 67:AG:71:VAL:HG22 | 1.85                     | 0.57              |
| 2:1:2669:A:H2'    | 2:1:2670:G:C8     | 2.39                     | 0.57              |
| 2:1:2873:G:O2'    | 2:1:2996:A:N1     | 2.37                     | 0.57              |
| 2:1:3144:A:O2'    | 57:w:6:LYS:NZ     | 2.36                     | 0.57              |
| 10:A:1263:G:OP1   | 14:E:186:LYS:NZ   | 2.37                     | 0.57              |
| 10:A:1445:C:OP2   | 27:T:138:THR:OG1  | 2.22                     | 0.57              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 27:T:16:ARG:HB2  | 53:s:116:TYR:HB3   | 1.86                     | 0.57              |
| 43:h:122:GLN:N   | 43:h:122:GLN:NE2   | 2.52                     | 0.57              |
| 54:t:168:ALA:HB1 | 62:AB:147:LEU:HD21 | 1.87                     | 0.57              |
| 58:x:122:ALA:HB3 | 58:x:143:PRO:HB2   | 1.85                     | 0.57              |
| 30:U:117:SER:HB3 | 30:U:123:ARG:HG3   | 1.87                     | 0.57              |
| 54:t:59:ARG:NH2  | 54:t:66:ASN:O      | 2.35                     | 0.57              |
| 78:AT:23:G:OP2   | 81:AT:101:GET:O31  | 2.14                     | 0.57              |
| 78:AT:51:U:O4    | 78:AT:65:G:O6      | 2.22                     | 0.57              |
| 2:1:1897:A:O2'   | 2:1:2890:G:OP1     | 2.18                     | 0.57              |
| 31:V:81:TYR:HB3  | 40:e:52:PHE:HB3    | 1.87                     | 0.57              |
| 2:1:1635:C:OP2   | 68:AH:74:ARG:NH1   | 2.34                     | 0.57              |
| 2:1:2380:A:H5''  | 46:l:68:THR:HG22   | 1.86                     | 0.57              |
| 2:1:3123:U:OP1   | 45:k:128:LYS:NZ    | 2.30                     | 0.57              |
| 5:4:8:C:H2'      | 5:4:9:A:H8         | 1.69                     | 0.57              |
| 10:A:12:U:H2'    | 10:A:13:C:C6       | 2.40                     | 0.57              |
| 10:A:378:U:C4    | 20:K:5:PRO:HB3     | 2.39                     | 0.57              |
| 10:A:903:U:H2'   | 10:A:904:A:C8      | 2.39                     | 0.57              |
| 17:H:7:TYR:HD1   | 17:H:113:ILE:HB    | 1.70                     | 0.57              |
| 35:Z:42:GLU:HG3  | 35:Z:52:LYS:HE3    | 1.86                     | 0.57              |
| 51:q:94:TYR:HA   | 51:q:177:ASP:OD1   | 2.05                     | 0.57              |
| 37:b:24:LEU:HD22 | 37:b:71:LEU:HD22   | 1.87                     | 0.57              |
| 43:h:189:PHE:HB3 | 43:h:220:TRP:CE2   | 2.40                     | 0.57              |
| 78:AT:69:C:H2'   | 78:AT:70:C:C6      | 2.40                     | 0.57              |
| 11:B:189:PRO:O   | 32:W:44:ARG:NH2    | 2.38                     | 0.57              |
| 20:K:106:GLU:OE1 | 20:K:115:LYS:NZ    | 2.37                     | 0.57              |
| 43:h:211:ALA:HB2 | 43:h:217:ILE:HG13  | 1.87                     | 0.57              |
| 65:AE:51:ASP:OD1 | 65:AE:91:TYR:OH    | 2.23                     | 0.57              |
| 9:9:51:ARG:HG2   | 9:9:52:GLN:H       | 1.70                     | 0.57              |
| 19:J:76:THR:HG21 | 19:J:104:ILE:HD12  | 1.86                     | 0.57              |
| 20:K:169:ALA:O   | 20:K:174:ARG:NH1   | 2.34                     | 0.57              |
| 49:o:108:GLN:NE2 | 49:o:204:LYS:HG2   | 2.20                     | 0.57              |
| 58:x:56:ARG:NH2  | 58:x:75:GLU:OE2    | 2.28                     | 0.57              |
| 72:AL:8:ILE:HD11 | 72:AL:65:LEU:HD13  | 1.87                     | 0.57              |
| 2:1:252:U:H5'    | 2:1:253:A:H8       | 1.70                     | 0.56              |
| 2:1:428:U:H2'    | 2:1:429:U:C6       | 2.39                     | 0.56              |
| 5:4:8:C:H2'      | 5:4:9:A:C8         | 2.40                     | 0.56              |
| 10:A:397:A:H4'   | 15:F:3:ARG:HG2     | 1.86                     | 0.56              |
| 13:D:32:PRO:HD3  | 13:D:41:LYS:NZ     | 2.20                     | 0.56              |
| 2:1:653:C:H2'    | 2:1:654:A:H8       | 1.69                     | 0.56              |
| 2:1:1106:U:H2'   | 2:1:1107:U:C6      | 2.40                     | 0.56              |
| 10:A:572:G:H4'   | 81:A:1804:GET:H231 | 1.87                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:A:850:A:OP1    | 33:X:28:ARG:NH2   | 2.33                     | 0.56              |
| 10:A:1593:C:H2'   | 10:A:1594:G:C8    | 2.40                     | 0.56              |
| 10:A:1745:U:O4    | 81:A:1801:GET:N12 | 2.38                     | 0.56              |
| 28:R:93:GLN:HE22  | 43:h:61:SER:HB2   | 1.69                     | 0.56              |
| 52:r:43:VAL:HG21  | 52:r:197:VAL:HG13 | 1.86                     | 0.56              |
| 66:AF:80:VAL:HG13 | 66:AF:112:LYS:HD2 | 1.87                     | 0.56              |
| 2:1:1692:A:H2'    | 2:1:1693:A:C8     | 2.40                     | 0.56              |
| 2:1:2421:A:O2'    | 2:1:2422:C:O5'    | 2.18                     | 0.56              |
| 2:1:2512:G:H2'    | 2:1:2513:A:C8     | 2.41                     | 0.56              |
| 2:1:3166:A:H2'    | 2:1:3167:G:C8     | 2.40                     | 0.56              |
| 10:A:215:A:H1'    | 10:A:216:A:N7     | 2.20                     | 0.56              |
| 10:A:317:U:H4'    | 10:A:321:A:C8     | 2.40                     | 0.56              |
| 10:A:1600:U:OP1   | 16:G:92:ARG:NH2   | 2.33                     | 0.56              |
| 11:B:60:ALA:O     | 11:B:64:ILE:HD12  | 2.05                     | 0.56              |
| 12:C:34:ALA:HB3   | 12:C:41:ARG:HA    | 1.86                     | 0.56              |
| 14:E:208:LYS:HB3  | 29:S:40:VAL:HB    | 1.86                     | 0.56              |
| 27:T:72:ILE:HG12  | 27:T:79:TYR:CD2   | 2.40                     | 0.56              |
| 28:R:81:ARG:HH11  | 28:R:115:LEU:HD23 | 1.71                     | 0.56              |
| 50:p:162:GLU:OE2  | 56:v:26:ARG:NH1   | 2.38                     | 0.56              |
| 76:AP:28:TYR:HB3  | 76:AP:69:VAL:HB   | 1.86                     | 0.56              |
| 10:A:219:A:H3'    | 10:A:818:U:N3     | 2.19                     | 0.56              |
| 26:Q:81:ARG:HB3   | 26:Q:117:GLY:HA3  | 1.88                     | 0.56              |
| 2:1:547:U:H2'     | 2:1:548:G:C8      | 2.40                     | 0.56              |
| 2:1:2810:A:N6     | 2:1:2822:G:O2'    | 2.39                     | 0.56              |
| 2:1:3144:A:OP1    | 67:AG:97:SER:OG   | 2.23                     | 0.56              |
| 17:H:49:ILE:HG13  | 17:H:114:VAL:HB   | 1.88                     | 0.56              |
| 42:g:161:ARG:NH1  | 42:g:181:GLN:OE1  | 2.39                     | 0.56              |
| 2:1:113:A:OP1     | 56:v:54:LYS:NZ    | 2.37                     | 0.56              |
| 2:1:1115:C:H2'    | 2:1:1116:A:C8     | 2.41                     | 0.56              |
| 6:6:38:ALA:HB3    | 6:6:59:MET:HB2    | 1.87                     | 0.56              |
| 10:A:1242:U:HO2'  | 21:L:8:ARG:HH21   | 1.54                     | 0.56              |
| 43:h:111:VAL:HG12 | 43:h:127:SER:HB2  | 1.86                     | 0.56              |
| 2:1:1653:C:O2'    | 2:1:1793:A:OP2    | 2.16                     | 0.56              |
| 2:1:2116:A:HO2'   | 71:AK:2:GLY:N     | 2.04                     | 0.56              |
| 4:3:23:A:H2'      | 4:3:24:A:C8       | 2.41                     | 0.56              |
| 10:A:277:G:H8     | 10:A:278:U:H5''   | 1.70                     | 0.56              |
| 10:A:826:U:H2'    | 10:A:827:C:C6     | 2.41                     | 0.56              |
| 10:A:1421:G:O6    | 21:L:64:TYR:OH    | 2.19                     | 0.56              |
| 10:A:1469:A:H2'   | 10:A:1470:G:C8    | 2.41                     | 0.56              |
| 43:h:94:ASP:N     | 43:h:99:GLU:O     | 2.38                     | 0.56              |
| 2:1:3248:U:H2'    | 2:1:3249:G:C8     | 2.41                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 18:I:14:GLU:OE2   | 18:I:42:ILE:N     | 2.38                     | 0.56              |
| 18:I:44:GLU:OE2   | 18:I:52:LYS:HE2   | 2.06                     | 0.56              |
| 37:b:26:CYS:SG    | 37:b:28:ARG:HB2   | 2.46                     | 0.56              |
| 42:g:182:TYR:HH   | 42:g:187:HIS:CG   | 2.24                     | 0.56              |
| 47:m:261:THR:OG1  | 47:m:264:GLN:OE1  | 2.15                     | 0.56              |
| 81:l:3409:GET:N33 | 4:3:90:A:OP1      | 2.39                     | 0.56              |
| 7:7:23:ARG:HG2    | 7:7:24:GLY:N      | 2.21                     | 0.56              |
| 10:A:1205:C:H2'   | 10:A:1206:A:C8    | 2.40                     | 0.56              |
| 11:B:198:MET:HG2  | 11:B:199:PRO:HD2  | 1.87                     | 0.56              |
| 12:C:223:PHE:HZ   | 12:C:228:LEU:HD22 | 1.70                     | 0.56              |
| 26:Q:103:ASN:HD22 | 26:Q:120:SER:HA   | 1.70                     | 0.56              |
| 51:q:93:VAL:HG22  | 74:AN:6:LEU:HD13  | 1.88                     | 0.56              |
| 53:s:18:VAL:HG22  | 53:s:70:THR:HG22  | 1.87                     | 0.56              |
| 3:2:56:TYR:CZ     | 3:2:78:LYS:HG3    | 2.41                     | 0.56              |
| 18:I:76:GLU:HA    | 18:I:79:LYS:HG2   | 1.87                     | 0.56              |
| 18:I:157:ALA:O    | 18:I:161:LYS:NZ   | 2.35                     | 0.56              |
| 41:f:29:LYS:HD3   | 41:f:30:PRO:HD2   | 1.87                     | 0.56              |
| 60:z:153:LYS:O    | 60:z:157:GLU:HG2  | 2.05                     | 0.56              |
| 2:1:2492:U:OP2    | 81:l:3413:GET:O41 | 2.24                     | 0.55              |
| 10:A:458:A:O2'    | 15:F:27:TYR:OH    | 2.19                     | 0.55              |
| 10:A:1155:G:C2    | 10:A:1156:A:C8    | 2.94                     | 0.55              |
| 10:A:1460:G:H2'   | 10:A:1461:A:C8    | 2.40                     | 0.55              |
| 13:D:58:VAL:HG11  | 13:D:64:ILE:HD11  | 1.89                     | 0.55              |
| 16:G:192:GLU:OE1  | 36:a:63:SER:OG    | 2.24                     | 0.55              |
| 35:Z:36:SER:HB3   | 35:Z:39:GLU:HG3   | 1.86                     | 0.55              |
| 43:h:237:VAL:HG22 | 43:h:253:THR:HG22 | 1.87                     | 0.55              |
| 78:AT:51:U:O2     | 78:AT:65:G:N2     | 2.34                     | 0.55              |
| 2:1:3319:U:N3     | 19:J:107:THR:OG1  | 2.26                     | 0.55              |
| 10:A:852:G:N2     | 24:O:87:ASP:OD1   | 2.37                     | 0.55              |
| 20:K:39:LYS:HD3   | 41:f:36:MET:HE1   | 1.87                     | 0.55              |
| 34:Y:70:LYS:HB3   | 34:Y:93:LEU:HD22  | 1.88                     | 0.55              |
| 46:l:6:GLN:HB3    | 46:l:20:GLN:HB3   | 1.88                     | 0.55              |
| 2:1:726:G:H5''    | 59:y:43:PRO:HB2   | 1.89                     | 0.55              |
| 2:1:820:C:H5''    | 44:j:21:ARG:HD3   | 1.88                     | 0.55              |
| 2:1:2420:G:H2'    | 2:1:2421:A:H5'    | 1.89                     | 0.55              |
| 10:A:1297:A:OP1   | 29:S:2:GLY:N      | 2.39                     | 0.55              |
| 10:A:1529:G:H22   | 10:A:1555:C:H1'   | 1.71                     | 0.55              |
| 16:G:58:LEU:HD11  | 16:G:167:ARG:NH1  | 2.22                     | 0.55              |
| 58:x:46:LYS:O     | 58:x:50:GLN:HG3   | 2.06                     | 0.55              |
| 10:A:933:A:H2'    | 10:A:934:C:C6     | 2.41                     | 0.55              |
| 10:A:1474:G:H3'   | 10:A:1502:A:H61   | 1.71                     | 0.55              |

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| Atom-1            | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 23:N:43:ARG:HB3   | 23:N:121:VAL:HG12   | 1.89                     | 0.55              |
| 34:Y:6:PRO:HG3    | 34:Y:14:LYS:HG2     | 1.89                     | 0.55              |
| 2:1:662:U:H2'     | 2:1:663:A:C8        | 2.41                     | 0.55              |
| 10:A:269:A:H61    | 17:H:185:GLN:HE22   | 1.54                     | 0.55              |
| 10:A:933:A:H2'    | 10:A:934:C:H6       | 1.71                     | 0.55              |
| 10:A:1167:U:H4'   | 26:Q:124:THR:HB     | 1.87                     | 0.55              |
| 15:F:107:GLY:HA2  | 15:F:189:LEU:HD23   | 1.89                     | 0.55              |
| 49:o:83:PHE:HB2   | 49:o:137:PRO:HG3    | 1.87                     | 0.55              |
| 49:o:185:GLU:HG2  | 49:o:196:VAL:HG21   | 1.87                     | 0.55              |
| 58:x:4:TYR:OH     | 58:x:18:ARG:HG3     | 2.06                     | 0.55              |
| 2:1:1762:G:O2'    | 2:1:1763:C:OP1      | 2.22                     | 0.55              |
| 2:1:2090:U:H4'    | 2:1:2091:A:O5'      | 2.07                     | 0.55              |
| 36:a:39:ILE:HB    | 36:a:71:ILE:HA      | 1.88                     | 0.55              |
| 43:h:239:ALA:HB3  | 43:h:252:ALA:HB3    | 1.89                     | 0.55              |
| 59:y:89:ASP:OD1   | 59:y:113[B]:ARG:NH1 | 2.39                     | 0.55              |
| 2:1:1589:A:OP1    | 68:AH:60:ARG:NH1    | 2.40                     | 0.55              |
| 10:A:160:A:H3'    | 10:A:161:G:H21      | 1.71                     | 0.55              |
| 10:A:723:G:H2'    | 10:A:724:G:H8       | 1.72                     | 0.55              |
| 10:A:1278:U:H3    | 10:A:1307:A:N6      | 1.99                     | 0.55              |
| 10:A:1773:G:OP2   | 25:P:128:ARG:NH2    | 2.39                     | 0.55              |
| 11:B:120:LEU:HD21 | 11:B:144:ILE:HD12   | 1.88                     | 0.55              |
| 12:C:133:TYR:HD2  | 12:C:217:LEU:HD11   | 1.72                     | 0.55              |
| 13:D:51:ILE:HA    | 13:D:56:LEU:HD12    | 1.88                     | 0.55              |
| 47:m:107:ARG:NH1  | 47:m:120:THR:O      | 2.39                     | 0.55              |
| 10:A:1239:U:H2'   | 10:A:1240:G:C8      | 2.41                     | 0.55              |
| 2:1:1530:A:H2'    | 2:1:1531:A:C8       | 2.42                     | 0.55              |
| 2:1:2527:G:N7     | 50:p:34:ASN:ND2     | 2.55                     | 0.55              |
| 2:1:3180:A:OP2    | 55:u:118:LYS:NZ     | 2.36                     | 0.55              |
| 13:D:165:ILE:HB   | 13:D:192:TYR:HB2    | 1.89                     | 0.55              |
| 16:G:156:ARG:CZ   | 39:d:67:ARG:HE      | 2.19                     | 0.55              |
| 20:K:106:GLU:HA   | 20:K:111:THR:HG21   | 1.87                     | 0.55              |
| 62:AB:60:TYR:HE2  | 62:AB:63:LYS:HA     | 1.72                     | 0.55              |
| 2:1:2852:U:H1'    | 45:k:250:ALA:HB3    | 1.89                     | 0.55              |
| 2:1:3193:C:H4'    | 2:1:3194:G:O5'      | 2.07                     | 0.55              |
| 2:1:3323:U:H2'    | 2:1:3324:A:H8       | 1.71                     | 0.55              |
| 5:4:21:C:OP1      | 46:l:194:LYS:NZ     | 2.34                     | 0.55              |
| 12:C:193:ILE:O    | 12:C:197:ILE:HG12   | 2.07                     | 0.55              |
| 27:T:76:PRO:HB2   | 27:T:86:LEU:HD21    | 1.88                     | 0.55              |
| 58:x:168:LEU:O    | 58:x:173:ARG:NH1    | 2.40                     | 0.55              |
| 2:1:2519:A:H1'    | 2:1:2520:A:OP2      | 2.07                     | 0.54              |
| 16:G:71:SER:O     | 16:G:91:GLU:HG2     | 2.07                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:T:38:VAL:HG13  | 27:T:42:TYR:HD2   | 1.71                     | 0.54              |
| 42:g:164:PRO:HD2  | 42:g:188:LEU:HD11 | 1.88                     | 0.54              |
| 46:l:301:ARG:HH21 | 59:y:41:ASP:HB3   | 1.72                     | 0.54              |
| 54:t:4:SER:O      | 62:AB:44:ASN:ND2  | 2.39                     | 0.54              |
| 59:y:178:ARG:HH21 | 62:AB:50:PRO:HG2  | 1.72                     | 0.54              |
| 2:1:3256:G:H2'    | 2:1:3257:A:H8     | 1.72                     | 0.54              |
| 10:A:308:C:H4'    | 34:Y:33:LEU:HD23  | 1.89                     | 0.54              |
| 13:D:40:VAL:HG21  | 13:D:63:ILE:HG23  | 1.89                     | 0.54              |
| 37:b:37:LYS:O     | 37:b:38:ARG:NH1   | 2.41                     | 0.54              |
| 38:c:35:VAL:HG11  | 38:c:63:LEU:HD13  | 1.88                     | 0.54              |
| 43:h:62:PHE:HZ    | 43:h:95:LEU:HA    | 1.72                     | 0.54              |
| 47:m:85:ARG:NH2   | 47:m:86:TYR:OH    | 2.41                     | 0.54              |
| 52:r:142:ASP:OD1  | 52:r:178:ARG:NH2  | 2.40                     | 0.54              |
| 56:v:105:ARG:HG2  | 56:v:108:ARG:HH21 | 1.73                     | 0.54              |
| 78:PT:64:G:H2'    | 78:PT:65:G:H8     | 1.72                     | 0.54              |
| 2:1:179:C:H2'     | 2:1:180:U:C6      | 2.42                     | 0.54              |
| 2:1:538:G:O2'     | 2:1:539:G:OP1     | 2.25                     | 0.54              |
| 2:1:1803:G:OP1    | 61:AA:133:LYS:NZ  | 2.38                     | 0.54              |
| 3:2:27:LEU:HD11   | 47:m:34:LYS:HA    | 1.90                     | 0.54              |
| 10:A:903:U:H2'    | 10:A:904:A:H8     | 1.71                     | 0.54              |
| 11:B:9:LEU:HD21   | 11:B:50:ILE:HG22  | 1.89                     | 0.54              |
| 30:U:29:GLU:N     | 30:U:110:LYS:HZ1  | 2.05                     | 0.54              |
| 44:j:80:GLU:HG3   | 77:AQ:66:GLY:HA2  | 1.88                     | 0.54              |
| 69:AI:50:ASN:OD1  | 69:AI:53:ARG:NH2  | 2.41                     | 0.54              |
| 10:A:215:A:H62    | 10:A:830:G:H1'    | 1.73                     | 0.54              |
| 10:A:529:C:O2'    | 10:A:530:U:OP1    | 2.24                     | 0.54              |
| 10:A:1512:A:H2'   | 10:A:1513:A:C8    | 2.42                     | 0.54              |
| 27:T:106:GLU:O    | 27:T:110:ARG:HG3  | 2.07                     | 0.54              |
| 46:l:93:ASN:HD22  | 46:l:101:PHE:HB2  | 1.72                     | 0.54              |
| 54:t:49:ARG:O     | 54:t:140:GLN:NE2  | 2.38                     | 0.54              |
| 2:1:2808:OMC:H5   | 2:1:2824:C:N4     | 2.06                     | 0.54              |
| 43:h:148:HIS:ND1  | 43:h:170:SER:HB2  | 2.23                     | 0.54              |
| 2:1:1493:C:H2'    | 2:1:1494:A:C8     | 2.43                     | 0.54              |
| 2:1:1592:C:H2'    | 2:1:1593:C:C6     | 2.42                     | 0.54              |
| 10:A:330:U:P      | 19:J:56:ARG:HH21  | 2.31                     | 0.54              |
| 10:A:1198:G:O2'   | 10:A:1229:A:N7    | 2.40                     | 0.54              |
| 10:A:1457:A:H2    | 10:A:1460:G:N3    | 2.05                     | 0.54              |
| 43:h:92:LEU:HD22  | 43:h:101:THR:HB   | 1.90                     | 0.54              |
| 60:z:105:LEU:HD22 | 60:z:135:LYS:HG3  | 1.90                     | 0.54              |
| 2:1:1204:U:H2'    | 74:AN:33:ASN:ND2  | 2.22                     | 0.54              |
| 2:1:3216:U:H2'    | 2:1:3217:G:C8     | 2.43                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:A:1511:A:H2'   | 10:A:1512:A:C8    | 2.43                     | 0.54              |
| 10:A:1529:G:N2    | 10:A:1556:A:OP2   | 2.39                     | 0.54              |
| 10:A:1784:A:N6    | 37:b:84:VAL:HB    | 2.23                     | 0.54              |
| 16:G:148:ARG:HA   | 16:G:157:ARG:HA   | 1.89                     | 0.54              |
| 20:K:126:ARG:HD3  | 41:f:33:ARG:HD3   | 1.90                     | 0.54              |
| 27:T:91:ASP:OD1   | 27:T:92:GLN:N     | 2.40                     | 0.54              |
| 36:a:83:LEU:HA    | 36:a:86:ASP:HB2   | 1.89                     | 0.54              |
| 52:r:38:ARG:NH1   | 52:r:83:ASP:O     | 2.40                     | 0.54              |
| 2:1:732:U:H3'     | 2:1:733:A:C8      | 2.42                     | 0.54              |
| 14:E:24:GLU:HG2   | 21:L:61:TRP:CD1   | 2.42                     | 0.54              |
| 46:l:218:LYS:HA   | 46:l:221:ARG:HG3  | 1.90                     | 0.54              |
| 6:6:77:ILE:HD12   | 6:6:103:VAL:HG11  | 1.90                     | 0.54              |
| 10:A:45:U:HO2'    | 10:A:46:A:H2'     | 1.71                     | 0.54              |
| 10:A:1311:A:H4'   | 14:E:157:PHE:CD1  | 2.43                     | 0.54              |
| 11:B:52:LYS:HG2   | 32:W:82:VAL:HG22  | 1.90                     | 0.54              |
| 27:T:52:VAL:HG11  | 27:T:61:LEU:HD11  | 1.89                     | 0.54              |
| 47:m:289:LYS:HA   | 47:m:292:GLU:HG2  | 1.91                     | 0.54              |
| 53:s:109:HIS:CD2  | 53:s:123:TYR:H    | 2.26                     | 0.54              |
| 1:0:90:MET:HE3    | 2:1:1209:G:H4'    | 1.90                     | 0.53              |
| 2:1:307:A:H2'     | 2:1:308:A:C8      | 2.43                     | 0.53              |
| 2:1:2974:C:O2'    | 45:k:180:GLU:OE2  | 2.24                     | 0.53              |
| 10:A:1314:A:OP2   | 14:E:161:SER:OG   | 2.18                     | 0.53              |
| 13:D:149:LEU:HD22 | 13:D:216:THR:HG21 | 1.91                     | 0.53              |
| 27:T:44:ASN:HD21  | 27:T:48:LYS:HE3   | 1.73                     | 0.53              |
| 32:W:71:ARG:O     | 32:W:75:GLN:HG3   | 2.08                     | 0.53              |
| 54:t:77:LEU:HD22  | 54:t:87:PRO:HG3   | 1.89                     | 0.53              |
| 76:AP:8:ARG:HG2   | 76:AP:10:THR:HG23 | 1.89                     | 0.53              |
| 2:1:1014:G:N2     | 2:1:1030:U:H3     | 2.01                     | 0.53              |
| 2:1:2347:G:H2'    | 2:1:2348:G:C8     | 2.42                     | 0.53              |
| 10:A:445:U:H2'    | 10:A:446:C:O4'    | 2.08                     | 0.53              |
| 12:C:87:ARG:HD2   | 12:C:101:HIS:HB2  | 1.89                     | 0.53              |
| 15:F:182:MET:HB2  | 15:F:228:ILE:HD13 | 1.91                     | 0.53              |
| 48:n:57:LEU:HD11  | 48:n:63:LEU:HB2   | 1.90                     | 0.53              |
| 10:A:189:G:H2'    | 10:A:190:U:H4'    | 1.90                     | 0.53              |
| 10:A:736:G:H2'    | 10:A:737:A:C8     | 2.43                     | 0.53              |
| 10:A:1571:G:C5    | 28:R:13:LYS:HE2   | 2.44                     | 0.53              |
| 10:A:1579:A:O2'   | 10:A:1580:A:OP1   | 2.25                     | 0.53              |
| 18:I:63:LEU:HD12  | 18:I:66:TYR:HB2   | 1.91                     | 0.53              |
| 28:R:47:VAL:HG12  | 28:R:81:ARG:HB3   | 1.90                     | 0.53              |
| 2:1:1113:G:OP1    | 63:AC:4:SER:HB2   | 2.08                     | 0.53              |
| 2:1:2985:U:H2'    | 2:1:2986:U:C6     | 2.44                     | 0.53              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 10:A:1699:G:H22   | 10:A:1700:G:N2   | 2.06                     | 0.53              |
| 27:T:83:ALA:O     | 27:T:89:GLN:NE2  | 2.41                     | 0.53              |
| 2:1:782:A:H4'     | 2:1:783:G:H5'    | 1.91                     | 0.53              |
| 2:1:1662:G:H2'    | 2:1:1663:A:C8    | 2.43                     | 0.53              |
| 6:6:10:LYS:NZ     | 6:6:54:ALA:O     | 2.41                     | 0.53              |
| 10:A:483:A:H2'    | 10:A:484:G:H8    | 1.72                     | 0.53              |
| 10:A:1233:C:H2'   | 10:A:1234:U:C5   | 2.43                     | 0.53              |
| 10:A:1571:G:O6    | 28:R:12:LYS:NZ   | 2.29                     | 0.53              |
| 16:G:77:TYR:HA    | 16:G:83:ARG:HG3  | 1.89                     | 0.53              |
| 43:h:21:THR:HA    | 43:h:287:ILE:HB  | 1.89                     | 0.53              |
| 43:h:67:HIS:CG    | 43:h:68:ILE:H    | 2.26                     | 0.53              |
| 53:s:109:HIS:HD2  | 53:s:123:TYR:H   | 1.56                     | 0.53              |
| 2:1:1663:A:H2'    | 2:1:1664:G:C8    | 2.44                     | 0.53              |
| 10:A:484:G:H1     | 10:A:499:U:H3    | 1.56                     | 0.53              |
| 10:A:1064:U:H2'   | 10:A:1065:U:C6   | 2.44                     | 0.53              |
| 16:G:197:GLU:OE2  | 16:G:208:SER:OG  | 2.22                     | 0.53              |
| 26:Q:30:THR:O     | 26:Q:34:THR:HG23 | 2.09                     | 0.53              |
| 26:Q:43:ARG:HE    | 26:Q:47:ARG:HD2  | 1.74                     | 0.53              |
| 43:h:292:SER:HB2  | 43:h:297:ASN:HB2 | 1.91                     | 0.53              |
| 51:q:69:ARG:NH1   | 51:q:73:SER:OG   | 2.41                     | 0.53              |
| 2:1:487:C:H2'     | 2:1:488:G:O4'    | 2.08                     | 0.53              |
| 2:1:972:U:OP1     | 59:y:144:ARG:NH2 | 2.37                     | 0.53              |
| 2:1:1189:A:OP1    | 57:w:50:ARG:NH2  | 2.33                     | 0.53              |
| 2:1:1782:G:H2'    | 2:1:1783:A:C8    | 2.44                     | 0.53              |
| 2:1:3287:A:H2'    | 2:1:3288:A:H8    | 1.74                     | 0.53              |
| 10:A:1042:U:H3'   | 10:A:1043:U:H3'  | 1.91                     | 0.53              |
| 10:A:1580:A:H2'   | 10:A:1581:G:C8   | 2.44                     | 0.53              |
| 2:1:437:G:O2'     | 2:1:438:A:OP1    | 2.27                     | 0.53              |
| 2:1:1173:G:C6     | 67:AG:20:LYS:HE2 | 2.44                     | 0.53              |
| 2:1:1774:G:O2'    | 2:1:1776:G:OP2   | 2.22                     | 0.53              |
| 2:1:2492:U:H5'    | 50:p:69:ARG:HG3  | 1.90                     | 0.53              |
| 2:1:2515:G:H4'    | 2:1:2516:U:OP1   | 2.09                     | 0.53              |
| 2:1:2749:G:C2     | 62:AB:60:TYR:CE1 | 2.97                     | 0.53              |
| 2:1:2869:A:H2'    | 2:1:2871:C:H5''  | 1.90                     | 0.53              |
| 10:A:405:A:H2'    | 10:A:406:C:H6    | 1.73                     | 0.53              |
| 14:E:124:LEU:HD23 | 14:E:155:ASP:HB2 | 1.90                     | 0.53              |
| 30:U:61:ILE:O     | 30:U:65:ILE:HD12 | 2.08                     | 0.53              |
| 45:k:284:ARG:NH1  | 45:k:293:ASN:O   | 2.42                     | 0.53              |
| 58:x:103:GLU:OE2  | 58:x:109:SER:OG  | 2.22                     | 0.53              |
| 2:1:2525:A:H2'    | 2:1:2526:C:O4'   | 2.09                     | 0.53              |
| 10:A:365:A:H2'    | 10:A:366:U:O4'   | 2.09                     | 0.53              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 10:A:1160:U:H2'   | 10:A:1161:G:C8     | 2.44                     | 0.53              |
| 10:A:1367:U:H1'   | 10:A:1503:A:N6     | 2.23                     | 0.53              |
| 10:A:1473:A:OP1   | 40:e:34:TYR:OH     | 2.13                     | 0.53              |
| 10:A:1699:G:H22   | 10:A:1700:G:H21    | 1.55                     | 0.53              |
| 29:S:84:TYR:HE1   | 29:S:86:PRO:HG3    | 1.74                     | 0.53              |
| 34:Y:3:LYS:HG3    | 34:Y:7:ARG:NH2     | 2.24                     | 0.53              |
| 34:Y:32:ARG:HG3   | 34:Y:33:LEU:HD12   | 1.91                     | 0.53              |
| 43:h:153:SER:HB3  | 43:h:171:TRP:CD1   | 2.44                     | 0.53              |
| 49:o:174:PHE:CZ   | 49:o:195:GLN:HG2   | 2.43                     | 0.53              |
| 58:x:165:GLN:OE1  | 58:x:166:ILE:N     | 2.40                     | 0.53              |
| 70:AJ:57:ILE:HD13 | 70:AJ:89:MET:HB3   | 1.90                     | 0.53              |
| 2:1:3315:C:O2'    | 2:1:3316:U:OP1     | 2.26                     | 0.53              |
| 6:6:75:PRO:HG2    | 6:6:105:PRO:HD3    | 1.91                     | 0.53              |
| 10:A:209:U:H5''   | 22:M:20:PHE:CG     | 2.44                     | 0.53              |
| 10:A:1226:G:H1'   | 26:Q:79:HIS:CD2    | 2.43                     | 0.53              |
| 13:D:64:ILE:HG21  | 13:D:131:ILE:HD12  | 1.91                     | 0.53              |
| 16:G:119:GLU:O    | 16:G:123:VAL:HG23  | 2.09                     | 0.53              |
| 19:J:142:SER:O    | 19:J:146:GLU:HG2   | 2.09                     | 0.53              |
| 27:T:18:LEU:HD13  | 27:T:66:LEU:HD12   | 1.89                     | 0.53              |
| 35:Z:89:TYR:CE2   | 35:Z:90:ARG:HG3    | 2.44                     | 0.53              |
| 36:a:95:HIS:CE1   | 36:a:97:LYS:HB2    | 2.44                     | 0.53              |
| 48:n:170:ARG:HB3  | 48:n:172:HIS:CE1   | 2.44                     | 0.53              |
| 60:z:60:ARG:O     | 60:z:64:ARG:HG3    | 2.09                     | 0.53              |
| 2:1:2536:U:H5''   | 50:p:41:ILE:HD12   | 1.90                     | 0.52              |
| 10:A:1131:G:H2'   | 10:A:1132:A:C8     | 2.43                     | 0.52              |
| 10:A:1240:G:H2'   | 23:N:47:GLU:OE2    | 2.09                     | 0.52              |
| 10:A:1281:A:OP1   | 11:B:138:TYR:OH    | 2.22                     | 0.52              |
| 10:A:1701:A:N1    | 10:A:1702:A:N6     | 2.58                     | 0.52              |
| 18:I:37:LEU:HD23  | 18:I:66:TYR:CD1    | 2.45                     | 0.52              |
| 18:I:135:ARG:HB3  | 33:X:51:GLU:OE2    | 2.09                     | 0.52              |
| 25:P:56:MET:HG2   | 25:P:99:ALA:HB2    | 1.90                     | 0.52              |
| 45:k:193:ASP:O    | 45:k:197:GLU:HG2   | 2.09                     | 0.52              |
| 46:l:42:ARG:HG2   | 46:l:112:VAL:HG11  | 1.90                     | 0.52              |
| 47:m:196:ARG:NH2  | 47:m:237:GLU:OE2   | 2.42                     | 0.52              |
| 2:1:252:U:H5'     | 2:1:253:A:C8       | 2.43                     | 0.52              |
| 10:A:1145:A:H2'   | 10:A:1146:C:H6     | 1.74                     | 0.52              |
| 10:A:1233:C:H2'   | 10:A:1234:U:H5     | 1.74                     | 0.52              |
| 54:t:76:THR:HG22  | 54:t:101:ARG:HB3   | 1.92                     | 0.52              |
| 2:1:1380:U:H5'    | 46:l:139:ARG:NH1   | 2.25                     | 0.52              |
| 2:1:1552:C:C5     | 81:1:3406:GET:H131 | 2.44                     | 0.52              |
| 3:2:112:ASN:OD1   | 3:2:128:LEU:HD13   | 2.09                     | 0.52              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 4:3:22:A:H2'      | 4:3:23:A:C8        | 2.44                     | 0.52              |
| 10:A:553:A:N3     | 10:A:588:C:O2'     | 2.41                     | 0.52              |
| 28:R:28:ILE:HD12  | 28:R:35:ILE:HG13   | 1.91                     | 0.52              |
| 52:r:66:GLU:OE2   | 52:r:69:ARG:NH2    | 2.36                     | 0.52              |
| 66:AF:77:VAL:HG13 | 66:AF:82:ASP:HB2   | 1.90                     | 0.52              |
| 2:1:805:G:OP1     | 81:1:3412:GET:N12  | 2.43                     | 0.52              |
| 2:1:2932:C:H2'    | 2:1:2933:G:H8      | 1.73                     | 0.52              |
| 2:1:3259:A:H2'    | 2:1:3260:A:O4'     | 2.09                     | 0.52              |
| 7:7:23:ARG:HG2    | 7:7:24:GLY:H       | 1.74                     | 0.52              |
| 10:A:561:U:H5     | 10:A:578:A:N7      | 2.07                     | 0.52              |
| 11:B:84:ARG:NH1   | 29:S:82:ASP:OD1    | 2.42                     | 0.52              |
| 12:C:168:MET:O    | 12:C:172:MET:HG3   | 2.10                     | 0.52              |
| 43:h:248:TRP:HZ3  | 43:h:259:ILE:HB    | 1.73                     | 0.52              |
| 48:n:44:GLY:O     | 48:n:47:ARG:NH1    | 2.34                     | 0.52              |
| 54:t:62:THR:HG23  | 62:AB:66:ASN:HB3   | 1.91                     | 0.52              |
| 2:1:1949:G:N1     | 2:1:2070:A:H2'     | 2.23                     | 0.52              |
| 2:1:2488:U:O2'    | 2:1:2489:A:H5''    | 2.10                     | 0.52              |
| 10:A:1242:U:O2'   | 21:L:8:ARG:NH2     | 2.34                     | 0.52              |
| 10:A:1540:G:N2    | 10:A:1542:A:H3'    | 2.24                     | 0.52              |
| 11:B:121:VAL:HG23 | 11:B:141:ILE:HG21  | 1.90                     | 0.52              |
| 13:D:50:GLN:HG3   | 13:D:234:PRO:HG3   | 1.91                     | 0.52              |
| 43:h:195:TYR:O    | 43:h:213:LYS:HB3   | 2.09                     | 0.52              |
| 2:1:368:G:H3'     | 81:1:3403:GET:H212 | 1.74                     | 0.52              |
| 2:1:2515:G:H1'    | 2:1:2516:U:O5'     | 2.09                     | 0.52              |
| 2:1:3248:U:H2'    | 2:1:3249:G:H8      | 1.75                     | 0.52              |
| 10:A:504:A:O2'    | 10:A:505:U:OP1     | 2.26                     | 0.52              |
| 10:A:675:U:H2'    | 10:A:676:G:C2      | 2.45                     | 0.52              |
| 11:B:190:ASP:OD1  | 11:B:191:ARG:N     | 2.39                     | 0.52              |
| 60:z:38:ARG:O     | 60:z:42:ARG:HG3    | 2.09                     | 0.52              |
| 61:AA:78:ASN:HA   | 64:AD:37:ARG:HH22  | 1.75                     | 0.52              |
| 2:1:1432:U:O4     | 46:l:68:THR:HG23   | 2.09                     | 0.52              |
| 2:1:2535:A:OP1    | 44:j:69:TYR:OH     | 2.24                     | 0.52              |
| 10:A:1463:G:H2'   | 10:A:1464:G:H8     | 1.74                     | 0.52              |
| 14:E:58:GLY:O     | 14:E:66:ARG:NH1    | 2.43                     | 0.52              |
| 14:E:60:LEU:HG    | 14:E:67:ILE:HD12   | 1.91                     | 0.52              |
| 26:Q:15:PHE:CE1   | 26:Q:110:GLU:HG3   | 2.45                     | 0.52              |
| 28:R:139:LYS:HE2  | 28:R:141:TYR:CE1   | 2.45                     | 0.52              |
| 42:g:163:CYS:HB3  | 42:g:168:CYS:SG    | 2.49                     | 0.52              |
| 2:1:163:A:H2'     | 2:1:164:U:H1'      | 1.92                     | 0.52              |
| 10:A:474:U:O4     | 20:K:37:LYS:NZ     | 2.43                     | 0.52              |
| 10:A:1246:G:H2'   | 10:A:1247:U:C6     | 2.45                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:P:73:ALA:HB2   | 25:P:106:ARG:HB2  | 1.92                     | 0.52              |
| 35:Z:29:HIS:NE2   | 35:Z:34:ASN:HA    | 2.25                     | 0.52              |
| 2:l:498:C:O2      | 48:n:22:LYS:HE3   | 2.10                     | 0.52              |
| 7:7:11:SER:HB2    | 45:k:369:ARG:HD2  | 1.92                     | 0.52              |
| 10:A:1348:U:H3'   | 10:A:1349:G:H8    | 1.75                     | 0.52              |
| 11:B:51:GLY:O     | 11:B:55:GLU:HG2   | 2.10                     | 0.52              |
| 14:E:6:LEU:HD12   | 14:E:10:LYS:HB3   | 1.92                     | 0.52              |
| 19:J:70:GLU:OE2   | 22:M:24:LYS:NZ    | 2.43                     | 0.52              |
| 44:j:4:VAL:HG13   | 44:j:8:GLN:OE1    | 2.10                     | 0.52              |
| 2:1:2917:G:O2'    | 2:1:2920:C:OP2    | 2.21                     | 0.52              |
| 10:A:1072:A:H2'   | 10:A:1073:A:C8    | 2.44                     | 0.52              |
| 10:A:1277:G:H21   | 11:B:111:ILE:HD11 | 1.74                     | 0.52              |
| 10:A:1566:U:H2'   | 10:A:1567:C:C6    | 2.45                     | 0.52              |
| 11:B:77:SER:HB2   | 11:B:124:THR:OG1  | 2.10                     | 0.52              |
| 16:G:166:ARG:HA   | 16:G:169:ASN:ND2  | 2.25                     | 0.52              |
| 27:T:103:ASN:HA   | 27:T:106:GLU:OE1  | 2.10                     | 0.52              |
| 38:c:45:THR:OG1   | 38:c:82:LYS:NZ    | 2.43                     | 0.52              |
| 79:MR:5:A:H2'     | 79:MR:6:A:C8      | 2.45                     | 0.52              |
| 2:1:299:G:H5''    | 70:AJ:84:ARG:NH2  | 2.25                     | 0.51              |
| 2:1:1199:A:H2'    | 2:1:1200:A:C8     | 2.45                     | 0.51              |
| 10:A:1129:U:H2'   | 10:A:1130:U:C6    | 2.45                     | 0.51              |
| 10:A:1209:A:H2'   | 10:A:1210:U:O4'   | 2.11                     | 0.51              |
| 17:H:98:ARG:NH2   | 17:H:105:ASP:OD1  | 2.39                     | 0.51              |
| 17:H:137:ARG:HB3  | 17:H:140:HIS:ND1  | 2.25                     | 0.51              |
| 28:R:20:HIS:HB2   | 28:R:65:ARG:HB2   | 1.91                     | 0.51              |
| 28:R:45:PHE:O     | 28:R:49:GLU:HG3   | 2.10                     | 0.51              |
| 47:m:194:LEU:HD12 | 47:m:197:LYS:HE3  | 1.92                     | 0.51              |
| 47:m:289:LYS:HD3  | 52:r:206:LEU:HD23 | 1.92                     | 0.51              |
| 61:AA:27:LYS:NZ   | 61:AA:93:LYS:O    | 2.43                     | 0.51              |
| 2:1:179:C:H2'     | 2:1:180:U:H6      | 1.75                     | 0.51              |
| 2:1:2384:C:H2'    | 2:1:2385:C:C6     | 2.45                     | 0.51              |
| 10:A:681:C:H2'    | 10:A:682:A:O4'    | 2.10                     | 0.51              |
| 10:A:1218:G:H22   | 10:A:1237:C:H5    | 1.58                     | 0.51              |
| 10:A:1369:G:O2'   | 10:A:1370:A:H8    | 1.92                     | 0.51              |
| 23:N:41:LEU:HD13  | 23:N:43:ARG:HD3   | 1.93                     | 0.51              |
| 27:T:84:TRP:HA    | 27:T:89:GLN:NE2   | 2.22                     | 0.51              |
| 28:R:12:LYS:CG    | 28:R:13:LYS:H     | 2.21                     | 0.51              |
| 28:R:98:GLU:HG2   | 43:h:60:LYS:HA    | 1.91                     | 0.51              |
| 35:Z:86:GLU:OE2   | 35:Z:90:ARG:NE    | 2.43                     | 0.51              |
| 43:h:172:ASP:OD1  | 43:h:174:THR:HB   | 2.09                     | 0.51              |
| 1:0:84:ARG:HD3    | 4:3:89:G:H4'      | 1.92                     | 0.51              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:1:229:C:H2'     | 2:1:230:G:O4'      | 2.10                     | 0.51              |
| 2:1:1216:U:O4     | 2:1:1282:A:O2'     | 2.24                     | 0.51              |
| 10:A:871:U:O2'    | 25:P:116:VAL:O     | 2.27                     | 0.51              |
| 10:A:1102:U:H2'   | 10:A:1103:G:C8     | 2.45                     | 0.51              |
| 10:A:1548:U:H2'   | 10:A:1549:G:H8     | 1.75                     | 0.51              |
| 11:B:144:ILE:HG12 | 11:B:158:VAL:HB    | 1.92                     | 0.51              |
| 42:g:186:CYS:O    | 42:g:187:HIS:ND1   | 2.44                     | 0.51              |
| 2:1:370:U:H4'     | 2:1:404:G:H5'      | 1.93                     | 0.51              |
| 2:1:599:U:C6      | 2:1:600:U:H5       | 2.28                     | 0.51              |
| 2:1:601:U:H3      | 49:o:25:ALA:HB1    | 1.75                     | 0.51              |
| 10:A:457:G:OP2    | 35:Z:105:ARG:NH2   | 2.43                     | 0.51              |
| 10:A:1289:G:H1'   | 10:A:1307:A:C2     | 2.45                     | 0.51              |
| 10:A:1431:G:N2    | 42:g:129:THR:OG1   | 2.42                     | 0.51              |
| 26:Q:81:ARG:NH2   | 26:Q:117:GLY:O     | 2.44                     | 0.51              |
| 31:V:33:LEU:HD21  | 31:V:88:ARG:HD3    | 1.92                     | 0.51              |
| 35:Z:23:PHE:CE1   | 35:Z:75:ILE:HG12   | 2.45                     | 0.51              |
| 42:g:147:TYR:HA   | 42:g:160:ARG:HH12  | 1.75                     | 0.51              |
| 67:AG:58:GLU:HG2  | 67:AG:63:LYS:HG3   | 1.93                     | 0.51              |
| 72:AL:49:ARG:HD3  | 72:AL:50:TYR:CE2   | 2.46                     | 0.51              |
| 2:1:406:G:O6      | 81:1:3403:GET:N32  | 2.39                     | 0.51              |
| 2:1:623:A:H2'     | 2:1:624:U:C6       | 2.45                     | 0.51              |
| 10:A:518:A:H2'    | 10:A:519:A:C8      | 2.45                     | 0.51              |
| 43:h:168:SER:OG   | 43:h:176:LYS:O     | 2.21                     | 0.51              |
| 61:AA:44:ALA:HB1  | 61:AA:114:VAL:HG21 | 1.92                     | 0.51              |
| 65:AE:5:ASP:O     | 65:AE:76:ARG:HD2   | 2.11                     | 0.51              |
| 2:1:3261:A:H2'    | 2:1:3262:U:H6      | 1.76                     | 0.51              |
| 10:A:897:U:H5''   | 10:A:899:G:O4'     | 2.11                     | 0.51              |
| 10:A:944:U:H5'    | 24:O:15:ALA:O      | 2.10                     | 0.51              |
| 10:A:1475:U:O2'   | 10:A:1501:A:N6     | 2.44                     | 0.51              |
| 10:A:1522:U:C4    | 16:G:187:ILE:HA    | 2.46                     | 0.51              |
| 27:T:129:TRP:HE3  | 27:T:131:LEU:HD12  | 1.75                     | 0.51              |
| 28:R:126:LYS:HE2  | 28:R:130:GLY:O     | 2.11                     | 0.51              |
| 28:R:141:TYR:O    | 28:R:142:ARG:HG2   | 2.11                     | 0.51              |
| 43:h:153:SER:H    | 43:h:170:SER:HA    | 1.76                     | 0.51              |
| 64:AD:29:TYR:OH   | 64:AD:57:GLU:OE2   | 2.29                     | 0.51              |
| 2:1:729:C:H3'     | 2:1:730:A:H5''     | 1.93                     | 0.51              |
| 2:1:1464:A:N1     | 2:1:1876:U:O2'     | 2.40                     | 0.51              |
| 7:7:11:SER:HB3    | 45:k:369:ARG:HH11  | 1.76                     | 0.51              |
| 10:A:1740:A:H2'   | 10:A:1741:A:C8     | 2.46                     | 0.51              |
| 12:C:164:VAL:O    | 12:C:168:MET:HG3   | 2.10                     | 0.51              |
| 43:h:25:THR:HG21  | 43:h:292:SER:HA    | 1.92                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 59:y:83:VAL:O     | 59:y:103:ALA:HA   | 2.11                     | 0.51              |
| 71:AK:76:ASN:O    | 71:AK:79:GLN:HG3  | 2.09                     | 0.51              |
| 78:AT:26:C:H2'    | 78:AT:27:G:O4'    | 2.11                     | 0.51              |
| 2:1:1104:U:H2'    | 2:1:1105:U:C6     | 2.45                     | 0.51              |
| 2:1:1344:U:O2     | 2:1:1347:U:O2'    | 2.26                     | 0.51              |
| 2:1:2790:U:H5'    | 2:1:2790:U:H6     | 1.75                     | 0.51              |
| 10:A:79:C:H5'     | 17:H:172:ALA:HB3  | 1.92                     | 0.51              |
| 10:A:857:G:H2'    | 10:A:858:U:O4'    | 2.11                     | 0.51              |
| 10:A:1436:U:H2'   | 10:A:1437:C:H6    | 1.76                     | 0.51              |
| 14:E:73:LEU:HA    | 21:L:20:VAL:HG11  | 1.92                     | 0.51              |
| 15:F:100:ARG:HH21 | 15:F:118:GLU:HG2  | 1.75                     | 0.51              |
| 17:H:164:LYS:HG3  | 17:H:167:LYS:HG3  | 1.93                     | 0.51              |
| 27:T:126:ARG:NH2  | 27:T:131:LEU:HB3  | 2.26                     | 0.51              |
| 28:R:12:LYS:HG2   | 28:R:75:SER:HA    | 1.93                     | 0.51              |
| 37:b:47:ALA:HA    | 37:b:50:VAL:HG23  | 1.93                     | 0.51              |
| 42:g:182:TYR:OH   | 42:g:187:HIS:CG   | 2.63                     | 0.51              |
| 2:1:941:C:H2'     | 2:1:942:U:C6      | 2.45                     | 0.51              |
| 2:1:2404:U:H2'    | 2:1:2405:U:C6     | 2.46                     | 0.51              |
| 10:A:810:U:H2'    | 10:A:811:U:C6     | 2.45                     | 0.51              |
| 10:A:924:A:H2'    | 10:A:925:A:C8     | 2.44                     | 0.51              |
| 10:A:1475:U:O2'   | 10:A:1476:A:H5''  | 2.09                     | 0.51              |
| 11:B:93:THR:HA    | 11:B:185:ARG:HH12 | 1.75                     | 0.51              |
| 14:E:114:LEU:HD22 | 14:E:119:ALA:HB2  | 1.92                     | 0.51              |
| 17:H:121:ILE:N    | 17:H:125:THR:OG1  | 2.39                     | 0.51              |
| 20:K:106:GLU:O    | 20:K:112:GLN:NE2  | 2.35                     | 0.51              |
| 27:T:65:GLU:O     | 27:T:69:ILE:HG12  | 2.11                     | 0.51              |
| 45:k:212:ASP:OD1  | 45:k:354:VAL:HG22 | 2.11                     | 0.51              |
| 2:1:1344:U:OP2    | 59:y:38:ARG:NH2   | 2.36                     | 0.51              |
| 2:1:2322:U:H2'    | 2:1:2323:A:C8     | 2.46                     | 0.51              |
| 10:A:108:A:H2'    | 10:A:109:G:C8     | 2.45                     | 0.51              |
| 10:A:723:G:H2'    | 10:A:724:G:C8     | 2.45                     | 0.51              |
| 10:A:840:A:H3'    | 10:A:841:A:H5''   | 1.93                     | 0.51              |
| 10:A:852:G:H21    | 24:O:87:ASP:CG    | 2.19                     | 0.51              |
| 10:A:1481:C:H2'   | 10:A:1482:C:C6    | 2.45                     | 0.51              |
| 10:A:1551:U:H2'   | 10:A:1552:C:C6    | 2.46                     | 0.51              |
| 10:A:1551:U:OP1   | 30:U:38:LYS:NZ    | 2.41                     | 0.51              |
| 42:g:185:LYS:O    | 42:g:186:CYS:HB3  | 2.11                     | 0.51              |
| 45:k:117:ARG:HD3  | 45:k:176:ALA:O    | 2.11                     | 0.51              |
| 2:1:2407:G:H2'    | 2:1:2408:A:C8     | 2.46                     | 0.50              |
| 10:A:119:A:H1'    | 10:A:395:A:C4     | 2.47                     | 0.50              |
| 10:A:184:C:H2'    | 10:A:185:G:O4'    | 2.10                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:A:1551:U:H2'   | 10:A:1552:C:H6    | 1.76                     | 0.50              |
| 10:A:1582:U:H5'   | 10:A:1583:C:OP2   | 2.11                     | 0.50              |
| 19:J:197:PHE:O    | 19:J:201:ARG:HG2  | 2.11                     | 0.50              |
| 30:U:29:GLU:H     | 30:U:110:LYS:NZ   | 2.07                     | 0.50              |
| 32:W:38:LYS:HG3   | 32:W:46:ILE:HD12  | 1.93                     | 0.50              |
| 54:t:64:LYS:HE3   | 62:AB:69:TRP:CD1  | 2.47                     | 0.50              |
| 73:AM:20:ASN:ND2  | 73:AM:42:ARG:O    | 2.38                     | 0.50              |
| 2:1:1794:A:H2'    | 2:1:1795:A:C8     | 2.47                     | 0.50              |
| 2:1:2171:U:H5'    | 2:1:2172:G:H5'    | 1.93                     | 0.50              |
| 2:1:3247:A:H2'    | 2:1:3248:U:C6     | 2.46                     | 0.50              |
| 10:A:1066:A:H1'   | 10:A:1067:C:O2    | 2.12                     | 0.50              |
| 10:A:1637:U:H2'   | 10:A:1638:A:C8    | 2.46                     | 0.50              |
| 11:B:84:ARG:NH1   | 29:S:82:ASP:O     | 2.45                     | 0.50              |
| 18:I:122:LEU:HD11 | 18:I:148:VAL:HG21 | 1.93                     | 0.50              |
| 20:K:62:ARG:HD3   | 20:K:66:ASP:OD2   | 2.11                     | 0.50              |
| 21:L:45:ALA:O     | 21:L:49:LEU:HG    | 2.11                     | 0.50              |
| 36:a:39:ILE:HG12  | 36:a:70:LYS:O     | 2.11                     | 0.50              |
| 43:h:70:GLN:HG2   | 43:h:112:LEU:HB2  | 1.92                     | 0.50              |
| 2:1:597:U:H2'     | 2:1:598:U:O4'     | 2.11                     | 0.50              |
| 10:A:1334:G:H2'   | 10:A:1335:U:C6    | 2.46                     | 0.50              |
| 13:D:135:ARG:HB2  | 13:D:217:TYR:CE1  | 2.47                     | 0.50              |
| 24:O:54:LEU:HB3   | 24:O:60:VAL:HB    | 1.92                     | 0.50              |
| 30:U:115:GLU:HG3  | 30:U:125:SER:HB3  | 1.93                     | 0.50              |
| 51:q:110:ASP:HB3  | 51:q:128:ILE:HD12 | 1.93                     | 0.50              |
| 78:AT:69:C:H2'    | 78:AT:70:C:H6     | 1.75                     | 0.50              |
| 10:A:207:U:H2'    | 10:A:208:A:C8     | 2.47                     | 0.50              |
| 10:A:884:G:O5'    | 25:P:41:MET:HG2   | 2.11                     | 0.50              |
| 11:B:18:LEU:HD12  | 11:B:23:HIS:CE1   | 2.47                     | 0.50              |
| 14:E:33:GLN:HG2   | 14:E:58:GLY:HA3   | 1.93                     | 0.50              |
| 16:G:135:ASP:HA   | 16:G:138:VAL:HG22 | 1.94                     | 0.50              |
| 17:H:164:LYS:HE3  | 17:H:167:LYS:HG3  | 1.94                     | 0.50              |
| 47:m:180:PHE:HB3  | 47:m:195:LEU:HD13 | 1.92                     | 0.50              |
| 2:1:1556:G:O2'    | 2:1:1557:U:H5'    | 2.11                     | 0.50              |
| 2:1:2405:U:H2'    | 2:1:2406:U:C6     | 2.46                     | 0.50              |
| 2:1:3323:U:H2'    | 2:1:3324:A:C8     | 2.45                     | 0.50              |
| 8:8:50:SER:HB2    | 69:AI:66:VAL:HG11 | 1.92                     | 0.50              |
| 10:A:753:C:H1'    | 20:K:143:ILE:HG21 | 1.94                     | 0.50              |
| 28:R:30:ILE:HG12  | 28:R:35:ILE:HD13  | 1.93                     | 0.50              |
| 43:h:16:HIS:NE2   | 43:h:35:SER:OG    | 2.30                     | 0.50              |
| 2:1:28:C:H4'      | 2:1:61:A:H4'      | 1.94                     | 0.50              |
| 2:1:429:U:H2'     | 2:1:430:G:H8      | 1.76                     | 0.50              |

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| Atom-1           | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|---------------------|--------------------------|-------------------|
| 2:1:495:C:H4'    | 48:n:79:ASN:HD21    | 1.77                     | 0.50              |
| 2:1:496:A:H2'    | 2:1:497:U:C6        | 2.47                     | 0.50              |
| 2:1:1684:U:H2'   | 2:1:1685:U:C5       | 2.47                     | 0.50              |
| 2:1:3245:A:O2'   | 2:1:3246:C:H6       | 1.95                     | 0.50              |
| 10:A:415:A:H4'   | 10:A:416:G:O5'      | 2.11                     | 0.50              |
| 10:A:1334:G:H2'  | 10:A:1335:U:H6      | 1.77                     | 0.50              |
| 10:A:1719:A:H2'  | 10:A:1720:C:C6      | 2.46                     | 0.50              |
| 43:h:93:TRP:HA   | 43:h:100:THR:HA     | 1.94                     | 0.50              |
| 2:1:907:C:H5''   | 44:j:15:ILE:HD13    | 1.93                     | 0.50              |
| 2:1:2158:A:H2'   | 2:1:2159:C:C6       | 2.46                     | 0.50              |
| 2:1:2734:A:H2'   | 2:1:2735:U:H6       | 1.77                     | 0.50              |
| 2:1:3019:U:O2'   | 2:1:3020:A:H5'      | 2.11                     | 0.50              |
| 24:O:100:LYS:O   | 24:O:103:GLU:HG2    | 2.12                     | 0.50              |
| 29:S:28:PHE:CE2  | 29:S:32:LYS:HD2     | 2.47                     | 0.50              |
| 31:V:47:TYR:HB2  | 31:V:49:ILE:HD12    | 1.93                     | 0.50              |
| 47:m:178:ASN:HA  | 47:m:183:TRP:CD2    | 2.47                     | 0.50              |
| 51:q:106:LYS:NZ  | 51:q:125:GLU:OE1    | 2.36                     | 0.50              |
| 59:y:89:ASP:OD1  | 59:y:113[A]:ARG:NH1 | 2.40                     | 0.50              |
| 69:AI:47:VAL:O   | 69:AI:51:ILE:HG13   | 2.12                     | 0.50              |
| 78:PT:24:C:H2'   | 78:PT:25:U:C6       | 2.46                     | 0.50              |
| 2:1:158:A:H2'    | 2:1:159:A:C8        | 2.47                     | 0.50              |
| 2:1:362:U:O4     | 71:AK:24:ARG:NH2    | 2.45                     | 0.50              |
| 2:1:1385:G:H5''  | 66:AF:102:SER:HB3   | 1.94                     | 0.50              |
| 2:1:2516:U:H5''  | 2:1:2517:C:C5       | 2.47                     | 0.50              |
| 2:1:2651:A:O2'   | 53:s:52:TYR:OH      | 2.05                     | 0.50              |
| 2:1:3182:C:C6    | 58:x:182:LEU:HD22   | 2.47                     | 0.50              |
| 10:A:391:C:H2'   | 10:A:392:C:C6       | 2.47                     | 0.50              |
| 10:A:1132:A:H2'  | 10:A:1133:C:C6      | 2.47                     | 0.50              |
| 48:n:50:ARG:HD3  | 48:n:158:TYR:CZ     | 2.47                     | 0.50              |
| 2:1:545:G:N2     | 2:1:546:C:O2'       | 2.45                     | 0.50              |
| 5:4:81:A:H2'     | 5:4:82:U:C6         | 2.47                     | 0.50              |
| 8:8:73:MET:HE1   | 8:8:142:ILE:HB      | 1.94                     | 0.50              |
| 10:A:72:A:H62    | 17:H:164:LYS:NZ     | 2.09                     | 0.50              |
| 10:A:503:A:H4'   | 10:A:504:A:OP1      | 2.11                     | 0.50              |
| 10:A:1699:G:N2   | 10:A:1700:G:N3      | 2.60                     | 0.50              |
| 11:B:167:LYS:HE2 | 11:B:203:PHE:HB3    | 1.94                     | 0.50              |
| 12:C:85:LYS:HG2  | 12:C:101:HIS:HB3    | 1.94                     | 0.50              |
| 12:C:88:VAL:HG21 | 12:C:96:LEU:HB2     | 1.94                     | 0.50              |
| 14:E:32:GLU:CD   | 14:E:32:GLU:H       | 2.19                     | 0.50              |
| 28:R:92:HIS:HA   | 28:R:96:VAL:HB      | 1.93                     | 0.50              |
| 35:Z:37:LYS:HD2  | 35:Z:57:VAL:HG23    | 1.93                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:1:1662:G:H2'     | 2:1:1663:A:H8      | 1.77                     | 0.49              |
| 2:1:2784:C:H2'     | 2:1:2785:A:H8      | 1.77                     | 0.49              |
| 81:1:3405:GET:H511 | 81:1:3405:GET:H322 | 1.77                     | 0.49              |
| 10:A:445:U:O2'     | 15:F:27:TYR:O      | 2.30                     | 0.49              |
| 10:A:520:U:H5''    | 35:Z:37:LYS:HG3    | 1.94                     | 0.49              |
| 10:A:1615:U:H2'    | 10:A:1616:G:C8     | 2.47                     | 0.49              |
| 13:D:234:PRO:HA    | 13:D:237:VAL:HG22  | 1.94                     | 0.49              |
| 15:F:103:TYR:HB2   | 15:F:182:MET:HE2   | 1.94                     | 0.49              |
| 18:I:27:GLN:O      | 18:I:31:LYS:HB2    | 2.12                     | 0.49              |
| 28:R:39:GLN:HB2    | 28:R:40:PRO:HD3    | 1.93                     | 0.49              |
| 2:1:11:A:H2'       | 2:1:12:A:C8        | 2.47                     | 0.49              |
| 2:1:2876:U:H2'     | 2:1:2877:U:C6      | 2.48                     | 0.49              |
| 2:1:3138:U:H2'     | 2:1:3139:U:C6      | 2.47                     | 0.49              |
| 2:1:3159:A:H2'     | 2:1:3160:C:C6      | 2.47                     | 0.49              |
| 10:A:1217:U:O4     | 42:g:137:HIS:NE2   | 2.40                     | 0.49              |
| 11:B:198:MET:HE3   | 29:S:85:VAL:HG13   | 1.94                     | 0.49              |
| 18:I:116:ALA:O     | 18:I:120:LYS:HG2   | 2.11                     | 0.49              |
| 20:K:110:GLN:NE2   | 20:K:126:ARG:HB2   | 2.26                     | 0.49              |
| 31:V:67:ARG:NH2    | 31:V:76:LYS:HD3    | 2.27                     | 0.49              |
| 2:1:563:U:H2'      | 2:1:564:G:C8       | 2.47                     | 0.49              |
| 2:1:1615:A:H2'     | 2:1:1616:U:O4'     | 2.12                     | 0.49              |
| 2:1:2544:U:H1'     | 2:1:2545:C:H6      | 1.77                     | 0.49              |
| 2:1:2784:C:H2'     | 2:1:2785:A:C8      | 2.48                     | 0.49              |
| 2:1:3261:A:H2'     | 2:1:3262:U:C6      | 2.48                     | 0.49              |
| 10:A:456:G:OP1     | 35:Z:109:LYS:NZ    | 2.44                     | 0.49              |
| 10:A:1309:G:H5'    | 11:B:113:ARG:HH22  | 1.77                     | 0.49              |
| 15:F:99:PHE:HE1    | 15:F:113:ARG:HE    | 1.59                     | 0.49              |
| 19:J:101:VAL:HG22  | 19:J:174:VAL:HG22  | 1.94                     | 0.49              |
| 31:V:44:ALA:HB3    | 31:V:51:LYS:HE3    | 1.93                     | 0.49              |
| 39:d:64:ARG:C      | 39:d:65:ARG:HD2    | 2.38                     | 0.49              |
| 78:PT:34:U:N3      | 78:PT:37:U:OP2     | 2.35                     | 0.49              |
| 2:1:72:A:N7        | 54:t:66:ASN:HB3    | 2.27                     | 0.49              |
| 2:1:694:C:H2'      | 2:1:695:G:C8       | 2.48                     | 0.49              |
| 6:6:15:LEU:HD13    | 6:6:51:ALA:HB3     | 1.94                     | 0.49              |
| 10:A:144:U:H5      | 10:A:166:A:N7      | 2.10                     | 0.49              |
| 10:A:1189:A:N3     | 40:e:10:HIS:NE2    | 2.53                     | 0.49              |
| 10:A:1604:U:H2'    | 10:A:1605:C:C6     | 2.47                     | 0.49              |
| 28:R:12:LYS:HG3    | 28:R:13:LYS:N      | 2.22                     | 0.49              |
| 39:d:28:VAL:N      | 39:d:42:ARG:O      | 2.31                     | 0.49              |
| 65:AE:45:THR:HG21  | 65:AE:89:PHE:HA    | 1.94                     | 0.49              |
| 2:1:1795:A:H2'     | 2:1:1796:A:C8      | 2.47                     | 0.49              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 2:1:2583:U:H2'     | 2:1:2584:U:C6     | 2.47                     | 0.49              |
| 2:1:2933:G:H2'     | 2:1:2934:U:C6     | 2.47                     | 0.49              |
| 2:1:3318:G:H3'     | 2:1:3319:U:H4'    | 1.95                     | 0.49              |
| 10:A:151:G:H2'     | 10:A:152:G:H8     | 1.76                     | 0.49              |
| 10:A:683:G:H2'     | 10:A:684:C:C6     | 2.46                     | 0.49              |
| 10:A:1741:A:C5     | 81:A:1801:GET:H21 | 2.48                     | 0.49              |
| 19:J:145:VAL:O     | 19:J:148:LYS:HG2  | 2.12                     | 0.49              |
| 20:K:127:VAL:CG1   | 20:K:131:GLN:HE22 | 2.26                     | 0.49              |
| 30:U:20:GLN:O      | 30:U:24:ARG:HG2   | 2.12                     | 0.49              |
| 30:U:107:ALA:O     | 30:U:111:ILE:HG12 | 2.12                     | 0.49              |
| 36:a:71:ILE:HB     | 36:a:75:LEU:HD22  | 1.95                     | 0.49              |
| 43:h:160:SER:HB3   | 43:h:205:GLY:HA3  | 1.93                     | 0.49              |
| 58:x:29:THR:HA     | 58:x:32:THR:HG22  | 1.94                     | 0.49              |
| 2:1:772:U:H5       | 2:1:2691:U:O2     | 1.95                     | 0.49              |
| 2:1:1543:G:H5''    | 56:v:108:ARG:NH1  | 2.27                     | 0.49              |
| 2:1:2741:A:O3'     | 76:AP:80:LYS:HB2  | 2.13                     | 0.49              |
| 2:1:3320:U:OP2     | 19:J:170:ARG:NH2  | 2.25                     | 0.49              |
| 5:4:26:U:H2'       | 5:4:27:U:C6       | 2.47                     | 0.49              |
| 10:A:116:U:H2'     | 10:A:117:U:C6     | 2.48                     | 0.49              |
| 10:A:194:G:H2'     | 10:A:195:A:O4'    | 2.13                     | 0.49              |
| 14:E:209:ILE:HG13  | 29:S:38:ILE:HG22  | 1.95                     | 0.49              |
| 25:P:37:VAL:HA     | 25:P:41:MET:CE    | 2.42                     | 0.49              |
| 25:P:117:PRO:HB3   | 25:P:120:SER:HB3  | 1.94                     | 0.49              |
| 27:T:88:ARG:HB3    | 27:T:98:TYR:O     | 2.12                     | 0.49              |
| 44:j:8:GLN:HE21    | 44:j:231:SER:C    | 2.20                     | 0.49              |
| 44:j:209:HIS:CE1   | 44:j:211:HIS:CD2  | 2.93                     | 0.49              |
| 2:1:437:G:H1       | 2:1:620:A:H62     | 1.59                     | 0.49              |
| 2:1:2072:C:H2'     | 2:1:2073:G:C8     | 2.48                     | 0.49              |
| 2:1:2870:G:N7      | 74:AN:49:LYS:HE3  | 2.27                     | 0.49              |
| 10:A:733:U:OP1     | 33:X:82:LYS:NZ    | 2.41                     | 0.49              |
| 10:A:892:A:H2'     | 10:A:893:U:C6     | 2.48                     | 0.49              |
| 11:B:169:SER:O     | 11:B:173:ILE:HG12 | 2.12                     | 0.49              |
| 13:D:133:PRO:HB2   | 13:D:217:TYR:HE2  | 1.78                     | 0.49              |
| 24:O:32:ASP:O      | 24:O:35:GLU:HG3   | 2.12                     | 0.49              |
| 30:U:116:ILE:HD13  | 30:U:122:ARG:HG2  | 1.95                     | 0.49              |
| 58:x:108:ASP:OD2   | 58:x:111:LYS:NZ   | 2.46                     | 0.49              |
| 1:0:138[A]:GLN:HG2 | 51:q:1:MET:HE1    | 1.95                     | 0.49              |
| 2:1:172:C:O2'      | 2:1:173:C:OP1     | 2.26                     | 0.49              |
| 2:1:261:U:H2'      | 2:1:262:U:C6      | 2.48                     | 0.49              |
| 9:9:27:ARG:HG2     | 9:9:78:PHE:CE1    | 2.48                     | 0.49              |
| 10:A:65:A:H2       | 10:A:84:A:H62     | 1.61                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:A:327:G:H5'    | 19:J:99:SER:HB2   | 1.95                     | 0.49              |
| 10:A:965:G:H4'    | 10:A:1763:A:H4'   | 1.95                     | 0.49              |
| 17:H:57:ASP:HA    | 17:H:106:LEU:HA   | 1.95                     | 0.49              |
| 23:N:32:LEU:HA    | 23:N:41:LEU:HD21  | 1.93                     | 0.49              |
| 26:Q:16:SER:O     | 27:T:93:VAL:HA    | 2.13                     | 0.49              |
| 43:h:91:ARG:HH21  | 43:h:100:THR:HG21 | 1.77                     | 0.49              |
| 52:r:42:THR:HG22  | 52:r:44:ASP:H     | 1.78                     | 0.49              |
| 54:t:126:PHE:HD2  | 69:AI:115:LYS:HG3 | 1.78                     | 0.49              |
| 1:0:164:GLN:HG2   | 1:0:166:THR:H     | 1.77                     | 0.49              |
| 2:1:842:A:N6      | 10:A:956:A:N1     | 2.61                     | 0.49              |
| 2:1:2079:C:HO2'   | 2:1:2080:U:H6     | 1.59                     | 0.49              |
| 10:A:82:U:H2'     | 10:A:83:G:O4'     | 2.12                     | 0.49              |
| 10:A:242:A:OP1    | 15:F:155:ARG:NE   | 2.46                     | 0.49              |
| 10:A:641:G:H2'    | 10:A:642:C:C6     | 2.48                     | 0.49              |
| 10:A:1479:A:H4'   | 10:A:1480:G:O5'   | 2.12                     | 0.49              |
| 12:C:225:LEU:HA   | 12:C:228:LEU:HB3  | 1.95                     | 0.49              |
| 28:R:98:GLU:O     | 28:R:101:LYS:HG2  | 2.13                     | 0.49              |
| 76:AP:7:THR:HB    | 76:AP:22:GLN:OE1  | 2.13                     | 0.49              |
| 78:PT:11:A:H2'    | 78:PT:12:G:C8     | 2.48                     | 0.49              |
| 1:0:42:TRP:CD1    | 1:0:53:LYS:HE2    | 2.48                     | 0.49              |
| 2:1:1286:A:H2'    | 2:1:1287:A:C8     | 2.48                     | 0.49              |
| 2:1:2130:A:H2'    | 2:1:2131:U:H6     | 1.78                     | 0.49              |
| 2:1:2655:U:H2'    | 2:1:2656:C:C6     | 2.47                     | 0.49              |
| 4:3:7:G:OP1       | 47:m:33:ARG:NH1   | 2.46                     | 0.49              |
| 4:3:97:A:O4'      | 49:o:222:GLN:NE2  | 2.46                     | 0.49              |
| 10:A:825:U:H1'    | 10:A:826:U:C2     | 2.48                     | 0.49              |
| 10:A:828:U:H2'    | 10:A:829:A:C8     | 2.48                     | 0.49              |
| 15:F:141:THR:OG1  | 15:F:143:ASP:OD1  | 2.26                     | 0.49              |
| 16:G:225:ARG:HG2  | 39:d:61:ARG:HH12  | 1.77                     | 0.49              |
| 17:H:63:MET:HE1   | 17:H:102:VAL:HG22 | 1.93                     | 0.49              |
| 17:H:162:VAL:HG21 | 17:H:171:LYS:HD2  | 1.95                     | 0.49              |
| 18:I:58:VAL:HG12  | 18:I:59:PRO:O     | 2.13                     | 0.49              |
| 2:1:25:A:H2'      | 2:1:26:C:H6       | 1.78                     | 0.48              |
| 2:1:248:U:H3'     | 2:1:249:G:H4'     | 1.94                     | 0.48              |
| 2:1:1172:C:H2'    | 2:1:1173:G:N2     | 2.28                     | 0.48              |
| 2:1:2669:A:H2'    | 2:1:2670:G:H8     | 1.78                     | 0.48              |
| 27:T:42:TYR:OH    | 27:T:73:MET:HA    | 2.12                     | 0.48              |
| 30:U:77:ASN:OD1   | 30:U:101:ASN:ND2  | 2.35                     | 0.48              |
| 36:a:63:SER:HA    | 36:a:66:VAL:HB    | 1.95                     | 0.48              |
| 2:1:58:G:H2'      | 5:4:33:A:O2'      | 2.13                     | 0.48              |
| 2:1:164:U:O2'     | 2:1:165:C:O5'     | 2.31                     | 0.48              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:1:1909:A:N3     | 2:1:2098:A:H2'     | 2.28                     | 0.48              |
| 2:1:2495:U:OP2    | 81:1:3406:GET:H932 | 2.14                     | 0.48              |
| 2:1:2653:U:H2'    | 2:1:2654:C:H6      | 1.78                     | 0.48              |
| 10:A:891:A:H2'    | 10:A:892:A:C8      | 2.48                     | 0.48              |
| 10:A:1343:G:H4'   | 30:U:130:ARG:HB2   | 1.95                     | 0.48              |
| 10:A:1375:C:H6    | 29:S:28:PHE:CE2    | 2.31                     | 0.48              |
| 10:A:1628:C:H2'   | 10:A:1629:G:C8     | 2.48                     | 0.48              |
| 11:B:62:ARG:HH21  | 32:W:38:LYS:HA     | 1.77                     | 0.48              |
| 17:H:10:ASN:HB3   | 17:H:128:THR:HA    | 1.94                     | 0.48              |
| 23:N:43:ARG:NH1   | 23:N:103:LEU:H     | 1.99                     | 0.48              |
| 54:t:169:TYR:CD2  | 62:AB:132:LYS:HG3  | 2.48                     | 0.48              |
| 2:1:538:G:N2      | 2:1:547:U:O2       | 2.45                     | 0.48              |
| 2:1:1493:C:H2'    | 2:1:1494:A:H8      | 1.78                     | 0.48              |
| 2:1:1616:U:H2'    | 2:1:1617:A:C8      | 2.48                     | 0.48              |
| 2:1:1684:U:H2'    | 2:1:1685:U:C6      | 2.49                     | 0.48              |
| 2:1:3183:A:H5''   | 2:1:3184:G:C5      | 2.48                     | 0.48              |
| 10:A:560:G:H2'    | 10:A:561:U:O2      | 2.13                     | 0.48              |
| 10:A:1238:U:O3'   | 42:g:185:LYS:HB2   | 2.13                     | 0.48              |
| 10:A:1580:A:H2'   | 10:A:1581:G:H8     | 1.79                     | 0.48              |
| 12:C:192:VAL:HA   | 12:C:195:ARG:HG2   | 1.96                     | 0.48              |
| 19:J:48:THR:HG21  | 19:J:54:LYS:HG3    | 1.95                     | 0.48              |
| 34:Y:107:PHE:CE2  | 34:Y:114:LYS:HB3   | 2.48                     | 0.48              |
| 36:a:64:VAL:HG13  | 36:a:68:ARG:HH11   | 1.78                     | 0.48              |
| 43:h:169:ALA:HA   | 43:h:175:VAL:HA    | 1.96                     | 0.48              |
| 47:m:153:THR:HG23 | 47:m:160:PHE:CZ    | 2.49                     | 0.48              |
| 53:s:136:ALA:HA   | 53:s:148:ILE:HD11  | 1.95                     | 0.48              |
| 75:AO:1:MET:O     | 75:AO:1:MET:HG2    | 2.13                     | 0.48              |
| 2:1:3165:U:H2'    | 2:1:3166:A:O4'     | 2.14                     | 0.48              |
| 10:A:697:U:H2'    | 10:A:698:C:C6      | 2.48                     | 0.48              |
| 10:A:787:A:C8     | 18:I:100:ARG:HG3   | 2.49                     | 0.48              |
| 10:A:1539:U:OP2   | 26:Q:43:ARG:NH2    | 2.34                     | 0.48              |
| 11:B:12:GLU:O     | 11:B:15:LYS:HB2    | 2.13                     | 0.48              |
| 11:B:16:LEU:HD13  | 11:B:175:TRP:HZ3   | 1.78                     | 0.48              |
| 2:1:583:A:H2'     | 2:1:584:C:C6       | 2.48                     | 0.48              |
| 2:1:2491:U:OP2    | 81:1:3413:GET:N32  | 2.47                     | 0.48              |
| 2:1:3183:A:H5''   | 2:1:3184:G:C4      | 2.49                     | 0.48              |
| 10:A:216:A:N1     | 10:A:829:A:H1'     | 2.28                     | 0.48              |
| 10:A:817:U:H3'    | 10:A:819:G:N7      | 2.29                     | 0.48              |
| 10:A:1048:U:H2'   | 10:A:1049:G:C8     | 2.49                     | 0.48              |
| 10:A:1566:U:H2'   | 10:A:1567:C:H6     | 1.79                     | 0.48              |
| 36:a:59:TYR:OH    | 36:a:61:SER:HB3    | 2.13                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:1:939:U:H3'      | 62:AB:13:GLY:HA2   | 1.96                     | 0.48              |
| 2:1:3230:C:OP2     | 48:n:69:LYS:NZ     | 2.38                     | 0.48              |
| 3:2:80:VAL:HB      | 3:2:83:ARG:NH1     | 2.27                     | 0.48              |
| 10:A:30:G:H2'      | 10:A:31:C:C6       | 2.48                     | 0.48              |
| 16:G:168:VAL:O     | 16:G:172:ILE:HD12  | 2.14                     | 0.48              |
| 43:h:22:SER:HB2    | 43:h:71:ASP:HA     | 1.95                     | 0.48              |
| 53:s:33:ALA:HA     | 53:s:36:VAL:HG12   | 1.95                     | 0.48              |
| 81:1:3413:GET:H111 | 81:1:3413:GET:O52  | 2.12                     | 0.48              |
| 10:A:199:G:O6      | 10:A:200:A:N6      | 2.46                     | 0.48              |
| 10:A:1495:U:H2'    | 10:A:1496:C:C6     | 2.48                     | 0.48              |
| 10:A:1668:A:H8     | 17:H:65:GLN:HG3    | 1.78                     | 0.48              |
| 11:B:84:ARG:NH2    | 11:B:201:LEU:HD12  | 2.29                     | 0.48              |
| 12:C:191:GLU:O     | 12:C:195:ARG:NE    | 2.45                     | 0.48              |
| 16:G:157:ARG:O     | 16:G:224:ASN:HB3   | 2.14                     | 0.48              |
| 26:Q:41:VAL:HG13   | 26:Q:84:ILE:HD13   | 1.95                     | 0.48              |
| 36:a:65:LEU:H      | 36:a:65:LEU:HD12   | 1.79                     | 0.48              |
| 59:y:123:THR:OG1   | 59:y:125:ASP:OD1   | 2.27                     | 0.48              |
| 2:1:29:G:OP1       | 56:v:172:ARG:HD2   | 2.13                     | 0.48              |
| 2:1:761:G:O6       | 54:t:182:LYS:NZ    | 2.34                     | 0.48              |
| 2:1:1093:G:H2'     | 2:1:1093:G:N3      | 2.29                     | 0.48              |
| 2:1:2634:G:H2'     | 2:1:2635:A:C8      | 2.48                     | 0.48              |
| 3:2:12:ARG:O       | 3:2:16:GLN:HG3     | 2.14                     | 0.48              |
| 10:A:193:G:H2'     | 10:A:194:G:C8      | 2.48                     | 0.48              |
| 10:A:446:C:H2'     | 10:A:447:C:C6      | 2.49                     | 0.48              |
| 10:A:1341:U:H2'    | 10:A:1342:A:C8     | 2.48                     | 0.48              |
| 81:A:1804:GET:H32  | 81:A:1804:GET:H111 | 1.57                     | 0.48              |
| 12:C:87:ARG:NH2    | 12:C:220:GLN:OE1   | 2.46                     | 0.48              |
| 18:I:30:LEU:HD13   | 18:I:72:ARG:HE     | 1.79                     | 0.48              |
| 19:J:67:TRP:CD2    | 19:J:70:GLU:HG3    | 2.49                     | 0.48              |
| 31:V:30:VAL:O      | 31:V:34:GLU:HG2    | 2.13                     | 0.48              |
| 39:d:64:ARG:HG2    | 39:d:65:ARG:N      | 2.27                     | 0.48              |
| 66:AF:14:TYR:CE2   | 66:AF:16:LYS:HB2   | 2.49                     | 0.48              |
| 2:1:2916:U:H1'     | 45:k:251:CYS:SG    | 2.54                     | 0.48              |
| 3:2:150:THR:OG1    | 46:l:363:ASN:HB2   | 2.13                     | 0.48              |
| 10:A:1589:C:H2'    | 10:A:1590:U:C6     | 2.49                     | 0.48              |
| 2:1:1380:U:H5'     | 46:l:139:ARG:HH12  | 1.78                     | 0.48              |
| 2:1:2260:U:OP1     | 2:1:2945:G:O2'     | 2.31                     | 0.48              |
| 2:1:2485:U:H2'     | 2:1:2486:U:C6      | 2.48                     | 0.48              |
| 10:A:1295:U:H2'    | 10:A:1296:U:C6     | 2.49                     | 0.48              |
| 11:B:201:LEU:O     | 11:B:202:TYR:HB2   | 2.14                     | 0.48              |
| 20:K:114:PHE:CE1   | 20:K:122:ILE:HD12  | 2.49                     | 0.48              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 26:Q:56:LEU:HD23 | 26:Q:83:MET:HE3   | 1.96                     | 0.48              |
| 29:S:60:ARG:NH2  | 29:S:66:VAL:HG21  | 2.28                     | 0.48              |
| 31:V:21:ILE:HG13 | 31:V:99:VAL:HG21  | 1.96                     | 0.48              |
| 35:Z:105:ARG:HG2 | 35:Z:109:LYS:HE2  | 1.96                     | 0.48              |
| 52:r:54:SER:HB2  | 52:r:135:ILE:HD11 | 1.94                     | 0.48              |
| 72:AL:77:ASN:C   | 72:AL:78:LEU:HD12 | 2.38                     | 0.48              |
| 2:1:1543:G:OP1   | 56:v:108:ARG:NH2  | 2.47                     | 0.47              |
| 2:1:2668:A:H2'   | 2:1:2669:A:C8     | 2.48                     | 0.47              |
| 2:1:2965:G:H2'   | 2:1:3114:A:N6     | 2.29                     | 0.47              |
| 5:4:63:G:O2'     | 69:AI:49:LYS:HE3  | 2.14                     | 0.47              |
| 7:7:35:LYS:HE3   | 7:7:51:TRP:CZ2    | 2.49                     | 0.47              |
| 10:A:74:U:O2'    | 10:A:75:U:O5'     | 2.32                     | 0.47              |
| 10:A:674:C:H2'   | 10:A:675:U:C6     | 2.48                     | 0.47              |
| 10:A:721:C:O2'   | 10:A:722:A:H5'    | 2.14                     | 0.47              |
| 10:A:829:A:H2'   | 10:A:830:G:C8     | 2.49                     | 0.47              |
| 10:A:899:G:O2'   | 10:A:900:A:N7     | 2.46                     | 0.47              |
| 15:F:45:VAL:HB   | 15:F:80:THR:HG22  | 1.95                     | 0.47              |
| 17:H:49:ILE:HG12 | 17:H:115:LYS:HB3  | 1.96                     | 0.47              |
| 39:d:27:GLN:OE1  | 39:d:43:ASN:HB3   | 2.13                     | 0.47              |
| 43:h:175:VAL:HB  | 43:h:189:PHE:HB2  | 1.96                     | 0.47              |
| 50:p:57:VAL:O    | 50:p:61:ARG:HG3   | 2.14                     | 0.47              |
| 51:q:48:ILE:HD11 | 51:q:54:LYS:HE3   | 1.94                     | 0.47              |
| 64:AD:28:GLY:O   | 64:AD:32:VAL:HG23 | 2.14                     | 0.47              |
| 70:AJ:3:LYS:HD2  | 70:AJ:12:LYS:O    | 2.14                     | 0.47              |
| 78:AT:44:A:H2'   | 78:AT:45:A:C8     | 2.49                     | 0.47              |
| 2:1:774:U:O4     | 81:1:3404:GET:N12 | 2.44                     | 0.47              |
| 2:1:2485:U:H2'   | 2:1:2486:U:H6     | 1.79                     | 0.47              |
| 10:A:1072:A:H5'  | 10:A:1283:U:C5    | 2.49                     | 0.47              |
| 10:A:1323:C:H1'  | 10:A:1396:A:C5    | 2.50                     | 0.47              |
| 13:D:143:LEU:O   | 13:D:169:ARG:NH2  | 2.45                     | 0.47              |
| 43:h:248:TRP:CZ3 | 43:h:259:ILE:HB   | 2.49                     | 0.47              |
| 55:u:27:ALA:HB2  | 55:u:45:ILE:HD13  | 1.96                     | 0.47              |
| 2:1:412:G:H2'    | 2:1:413:U:C6      | 2.49                     | 0.47              |
| 2:1:2899:C:H2'   | 2:1:2900:C:C6     | 2.49                     | 0.47              |
| 5:4:5:U:H2'      | 5:4:6:U:C6        | 2.48                     | 0.47              |
| 5:4:85:G:H4'     | 5:4:86:U:OP1      | 2.14                     | 0.47              |
| 10:A:16:G:H2'    | 10:A:17:C:C6      | 2.48                     | 0.47              |
| 10:A:932:U:H2'   | 10:A:933:A:C8     | 2.50                     | 0.47              |
| 10:A:944:U:H5''  | 24:O:14:SER:OG    | 2.14                     | 0.47              |
| 10:A:1007:C:O2'  | 10:A:1110:A:N1    | 2.45                     | 0.47              |
| 10:A:1431:G:N1   | 42:g:129:THR:O    | 2.34                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:G:121:ILE:O    | 16:G:125:THR:HG22 | 2.14                     | 0.47              |
| 30:U:38:LYS:HE3   | 30:U:40:SER:O     | 2.14                     | 0.47              |
| 41:f:13:LYS:O     | 41:f:17:GLN:HG2   | 2.14                     | 0.47              |
| 44:j:30:ARG:O     | 44:j:163:ARG:NH1  | 2.42                     | 0.47              |
| 70:AJ:95:GLU:HA   | 70:AJ:98:ARG:HG2  | 1.97                     | 0.47              |
| 2:1:208:A:H4'     | 2:1:210:A:N7      | 2.30                     | 0.47              |
| 10:A:103:A:H4'    | 10:A:105:A:C8     | 2.49                     | 0.47              |
| 10:A:214:U:O2'    | 10:A:215:A:OP1    | 2.28                     | 0.47              |
| 10:A:836:U:H2'    | 10:A:837:C:O4'    | 2.14                     | 0.47              |
| 11:B:41:ARG:CZ    | 11:B:45:MET:HB2   | 2.45                     | 0.47              |
| 17:H:31:ARG:HB3   | 17:H:34:GLN:HG3   | 1.95                     | 0.47              |
| 20:K:20:GLU:HB2   | 20:K:23:ARG:HG2   | 1.97                     | 0.47              |
| 22:M:17:PRO:O     | 22:M:19:ILE:HD12  | 2.14                     | 0.47              |
| 42:g:182:TYR:CE1  | 42:g:187:HIS:HB3  | 2.49                     | 0.47              |
| 70:AJ:60:ILE:HG21 | 70:AJ:90:THR:HG22 | 1.95                     | 0.47              |
| 2:1:589:G:O2'     | 48:n:16:ALA:O     | 2.31                     | 0.47              |
| 2:1:2397:A:H2'    | 2:1:2398:C:C6     | 2.50                     | 0.47              |
| 2:1:2546:U:H5'    | 2:1:2547:G:C8     | 2.48                     | 0.47              |
| 2:1:2646:A:C2     | 53:s:124:GLY:HA3  | 2.49                     | 0.47              |
| 10:A:393:U:H2'    | 10:A:394:G:O4'    | 2.15                     | 0.47              |
| 10:A:1311:A:H4'   | 14:E:157:PHE:CE1  | 2.49                     | 0.47              |
| 10:A:1719:A:H2'   | 10:A:1720:C:H6    | 1.78                     | 0.47              |
| 11:B:75:VAL:HG12  | 11:B:122:VAL:HB   | 1.97                     | 0.47              |
| 12:C:72:ASP:OD1   | 37:b:59:TYR:OH    | 2.24                     | 0.47              |
| 16:G:21:GLN:HG2   | 16:G:21:GLN:O     | 2.15                     | 0.47              |
| 16:G:51:VAL:HG22  | 16:G:131:GLN:HB2  | 1.95                     | 0.47              |
| 48:n:57:LEU:CD1   | 48:n:63:LEU:HB2   | 2.45                     | 0.47              |
| 49:o:32:LYS:HE2   | 49:o:32:LYS:HB2   | 1.59                     | 0.47              |
| 60:z:86:ASP:OD1   | 60:z:90:PRO:HA    | 2.14                     | 0.47              |
| 2:1:2527:G:C5     | 50:p:34:ASN:ND2   | 2.82                     | 0.47              |
| 2:1:2862:A:O2'    | 2:1:2905:A:N3     | 2.45                     | 0.47              |
| 2:1:3256:G:H2'    | 2:1:3257:A:C8     | 2.50                     | 0.47              |
| 9:9:58:VAL:HA     | 9:9:104:VAL:HG12  | 1.96                     | 0.47              |
| 10:A:485:G:N1     | 10:A:499:U:O4     | 2.46                     | 0.47              |
| 10:A:952:A:OP2    | 24:O:124:ARG:NH2  | 2.36                     | 0.47              |
| 10:A:1635:A:H2'   | 10:A:1636:C:C6    | 2.49                     | 0.47              |
| 13:D:135:ARG:HD2  | 13:D:217:TYR:CE1  | 2.49                     | 0.47              |
| 20:K:34:TYR:HA    | 20:K:122:ILE:HD13 | 1.96                     | 0.47              |
| 27:T:67:GLU:O     | 27:T:71:THR:HG23  | 2.14                     | 0.47              |
| 32:W:39:VAL:HG12  | 32:W:40:ASP:O     | 2.14                     | 0.47              |
| 55:u:17:ARG:HG2   | 55:u:57:LEU:HD22  | 1.97                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 62:AB:19:LYS:HB3  | 62:AB:25:HIS:HB2  | 1.96                     | 0.47              |
| 65:AE:78:ARG:HA   | 65:AE:88:LEU:HD23 | 1.96                     | 0.47              |
| 72:AL:43:PHE:HE1  | 72:AL:66:GLN:HG2  | 1.79                     | 0.47              |
| 2:1:602:A:OP2     | 2:1:602:A:H8      | 1.98                     | 0.47              |
| 2:1:1058:A:H4'    | 3:2:105:PHE:CE1   | 2.49                     | 0.47              |
| 2:1:1080:A:H2'    | 2:1:1081:A:C8     | 2.49                     | 0.47              |
| 2:1:1190:G:H2'    | 2:1:1191:A:C8     | 2.49                     | 0.47              |
| 2:1:1655:U:H2'    | 2:1:1656:C:C6     | 2.49                     | 0.47              |
| 2:1:1911:A:H2'    | 2:1:1912:U:C6     | 2.50                     | 0.47              |
| 2:1:2116:A:C4     | 71:AK:3:LYS:HB3   | 2.49                     | 0.47              |
| 2:1:2385:C:H2'    | 2:1:2386:U:C6     | 2.50                     | 0.47              |
| 2:1:2527:G:C8     | 50:p:34:ASN:ND2   | 2.82                     | 0.47              |
| 2:1:2876:U:H2'    | 2:1:2877:U:H6     | 1.80                     | 0.47              |
| 2:1:3260:A:H2'    | 2:1:3261:A:H8     | 1.79                     | 0.47              |
| 3:2:39:ILE:HD12   | 3:2:102:ARG:CD    | 2.45                     | 0.47              |
| 10:A:653:G:H4'    | 10:A:654:G:H5'    | 1.95                     | 0.47              |
| 10:A:876:A:O2'    | 10:A:877:G:OP1    | 2.24                     | 0.47              |
| 10:A:1205:C:H2'   | 10:A:1206:A:H8    | 1.77                     | 0.47              |
| 10:A:1374:A:H61   | 10:A:1395:G:H21   | 1.62                     | 0.47              |
| 16:G:166:ARG:HG2  | 16:G:170:GLN:OE1  | 2.14                     | 0.47              |
| 16:G:194:LEU:O    | 16:G:198:LEU:HG   | 2.13                     | 0.47              |
| 17:H:20:ASP:OD1   | 17:H:22:HIS:ND1   | 2.47                     | 0.47              |
| 26:Q:119:PHE:HE1  | 27:T:119:ILE:HD12 | 1.80                     | 0.47              |
| 27:T:20:THR:O     | 27:T:22:ILE:N     | 2.48                     | 0.47              |
| 27:T:41:ARG:HH11  | 30:U:46:PRO:HD3   | 1.79                     | 0.47              |
| 27:T:58:ALA:HA    | 27:T:61:LEU:HD23  | 1.97                     | 0.47              |
| 28:R:20:HIS:N     | 28:R:65:ARG:O     | 2.47                     | 0.47              |
| 30:U:14:PHE:HZ    | 30:U:132:LEU:HD12 | 1.80                     | 0.47              |
| 31:V:98:THR:O     | 31:V:102:ILE:HG12 | 2.14                     | 0.47              |
| 46:l:301:ARG:NH2  | 59:y:41:ASP:HB3   | 2.29                     | 0.47              |
| 53:s:83:GLY:HA3   | 53:s:127:PHE:HE2  | 1.80                     | 0.47              |
| 60:z:134:HIS:CD2  | 60:z:136:ARG:HB3  | 2.50                     | 0.47              |
| 2:1:2260:U:O2     | 2:1:2288:U:H4'    | 2.15                     | 0.47              |
| 2:1:2825:A:H1'    | 52:r:158:LYS:HD2  | 1.96                     | 0.47              |
| 10:A:1575:G:N2    | 10:A:1595:U:O2    | 2.33                     | 0.47              |
| 17:H:157:VAL:HG21 | 17:H:175:ILE:HD11 | 1.96                     | 0.47              |
| 18:I:113:THR:O    | 18:I:117:VAL:HG23 | 2.15                     | 0.47              |
| 21:L:46:LEU:O     | 21:L:50:THR:HG23  | 2.14                     | 0.47              |
| 33:X:15:ASN:ND2   | 33:X:71:LYS:HD2   | 2.30                     | 0.47              |
| 43:h:304:ASP:CG   | 43:h:308:ARG:HH12 | 2.23                     | 0.47              |
| 53:s:137:ARG:O    | 53:s:141:ARG:HG2  | 2.15                     | 0.47              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:1:1625:U:O4     | 61:AA:111:LYS:HE3  | 2.15                     | 0.47              |
| 2:1:1756:A:C6     | 2:1:1762:G:C6      | 3.03                     | 0.47              |
| 2:1:2421:A:HO2'   | 2:1:2422:C:P       | 2.37                     | 0.47              |
| 2:1:2647:C:H42    | 53:s:22:CYS:HB3    | 1.79                     | 0.47              |
| 2:1:2686:G:H4'    | 2:1:2687:A:H5''    | 1.95                     | 0.47              |
| 2:1:3009:U:H5''   | 45:k:348:ARG:HE    | 1.79                     | 0.47              |
| 16:G:46:TRP:CZ2   | 16:G:118:LEU:HB3   | 2.50                     | 0.47              |
| 16:G:162:VAL:HG13 | 16:G:166:ARG:HD3   | 1.96                     | 0.47              |
| 17:H:159:ARG:HG2  | 17:H:172:ALA:HB2   | 1.97                     | 0.47              |
| 17:H:191:LYS:O    | 17:H:195:VAL:HG23  | 2.15                     | 0.47              |
| 38:c:33:MET:HB2   | 38:c:79:PHE:HB2    | 1.97                     | 0.47              |
| 53:s:60:ARG:HE    | 76:AP:103:ALA:HB1  | 1.80                     | 0.47              |
| 56:v:115:VAL:HA   | 56:v:134:LEU:HD23  | 1.97                     | 0.47              |
| 2:1:612:U:H2'     | 2:1:613:U:C6       | 2.50                     | 0.47              |
| 2:1:631:U:H2'     | 2:1:632:C:C6       | 2.50                     | 0.47              |
| 2:1:2995:U:H2'    | 2:1:2996:A:H8      | 1.79                     | 0.47              |
| 10:A:1437:C:H2'   | 10:A:1438:U:H6     | 1.80                     | 0.47              |
| 13:D:85:THR:OG1   | 13:D:88:GLY:O      | 2.23                     | 0.47              |
| 13:D:135:ARG:HB3  | 13:D:216:THR:HB    | 1.96                     | 0.47              |
| 21:L:1:MET:HE1    | 21:L:40:LEU:HG     | 1.97                     | 0.47              |
| 27:T:41:ARG:HH22  | 30:U:37:VAL:C      | 2.23                     | 0.47              |
| 37:b:39:VAL:HG22  | 37:b:70:LYS:HG3    | 1.97                     | 0.47              |
| 43:h:254:THR:HA   | 43:h:285:GLU:CD    | 2.40                     | 0.47              |
| 49:o:158:ARG:HG3  | 49:o:201:TRP:CD2   | 2.49                     | 0.47              |
| 2:1:2960:C:OP1    | 57:w:69:LYS:HE2    | 2.14                     | 0.46              |
| 3:2:40:VAL:HB     | 3:2:96:VAL:HG13    | 1.97                     | 0.46              |
| 10:A:260:U:C2'    | 10:A:261:C:H5'     | 2.44                     | 0.46              |
| 10:A:1357:A:C2    | 10:A:1359:U:H1'    | 2.51                     | 0.46              |
| 10:A:1673:U:C6    | 10:A:1704:C:H1'    | 2.49                     | 0.46              |
| 12:C:156:ALA:HB3  | 12:C:161:LEU:HD21  | 1.97                     | 0.46              |
| 18:I:126:VAL:HB   | 18:I:129:THR:OG1   | 2.14                     | 0.46              |
| 26:Q:18:LYS:HD3   | 27:T:91:ASP:O      | 2.16                     | 0.46              |
| 39:d:42:ARG:HG3   | 39:d:43:ASN:H      | 1.80                     | 0.46              |
| 42:g:163:CYS:SG   | 42:g:186:CYS:SG    | 3.09                     | 0.46              |
| 65:AE:73:ARG:NH1  | 65:AE:108:VAL:HG11 | 2.30                     | 0.46              |
| 2:1:72:A:C4       | 70:AJ:14:ARG:HD2   | 2.51                     | 0.46              |
| 2:1:2181:U:H2'    | 2:1:2182:C:C6      | 2.50                     | 0.46              |
| 2:1:3202:U:H2'    | 2:1:3203:A:C8      | 2.50                     | 0.46              |
| 5:4:78:G:H2'      | 5:4:79:A:C2        | 2.49                     | 0.46              |
| 10:A:691:U:H5'    | 10:A:692:U:C5'     | 2.43                     | 0.46              |
| 20:K:112:GLN:HB3  | 20:K:153:GLN:HE22  | 1.80                     | 0.46              |

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| Atom-1               | Atom-2               | Interatomic distance (Å) | Clash overlap (Å) |
|----------------------|----------------------|--------------------------|-------------------|
| 43:h:286:ALA:HB2     | 43:h:302:TYR:CD1     | 2.50                     | 0.46              |
| 68:AH:106[B]:LYS:HB3 | 68:AH:106[B]:LYS:HE3 | 1.61                     | 0.46              |
| 78:PT:67:C:H2'       | 78:PT:68:C:H6        | 1.79                     | 0.46              |
| 2:1:1762:G:HO2'      | 2:1:1763:C:P         | 2.38                     | 0.46              |
| 10:A:528:C:O2        | 35:Z:61:ARG:NH1      | 2.32                     | 0.46              |
| 10:A:530:U:P         | 35:Z:65:GLY:H        | 2.39                     | 0.46              |
| 10:A:1512:A:H2'      | 10:A:1513:A:H8       | 1.79                     | 0.46              |
| 16:G:58:LEU:HD11     | 16:G:167:ARG:HH12    | 1.79                     | 0.46              |
| 20:K:110:GLN:NE2     | 20:K:122:ILE:HG12    | 2.30                     | 0.46              |
| 29:S:24:LEU:HB2      | 29:S:58:MET:HE3      | 1.97                     | 0.46              |
| 30:U:105:VAL:O       | 30:U:109:GLN:HG2     | 2.16                     | 0.46              |
| 66:AF:17[A]:LYS:HB3  | 66:AF:17[A]:LYS:HE3  | 1.55                     | 0.46              |
| 2:1:293:C:H2'        | 2:1:294:U:O4'        | 2.16                     | 0.46              |
| 2:1:3322:U:H2'       | 2:1:3323:U:C6        | 2.50                     | 0.46              |
| 10:A:1039:U:H2'      | 10:A:1040:U:C6       | 2.50                     | 0.46              |
| 10:A:1300:U:O2'      | 10:A:1301:G:H8       | 1.99                     | 0.46              |
| 10:A:1302:C:H2'      | 10:A:1303:G:O4'      | 2.15                     | 0.46              |
| 10:A:1317:C:O2'      | 14:E:163:GLN:HB3     | 2.16                     | 0.46              |
| 26:Q:94:VAL:HG21     | 26:Q:116:LEU:HD21    | 1.97                     | 0.46              |
| 30:U:14:PHE:CZ       | 30:U:132:LEU:HD12    | 2.50                     | 0.46              |
| 44:j:32:LEU:HD11     | 44:j:120:VAL:HG22    | 1.98                     | 0.46              |
| 45:k:283:TYR:OH      | 45:k:325:LYS:HD2     | 2.15                     | 0.46              |
| 51:q:18:VAL:HG22     | 51:q:27:VAL:HG13     | 1.96                     | 0.46              |
| 72:AL:24:ILE:HB      | 72:AL:44:LYS:HB2     | 1.97                     | 0.46              |
| 1:0:43:TYR:CZ        | 1:0:47:LYS:HE2       | 2.50                     | 0.46              |
| 2:1:264:G:OP1        | 70:AJ:34:GLN:HG2     | 2.16                     | 0.46              |
| 2:1:2335:A:H2'       | 2:1:2336:A:C8        | 2.50                     | 0.46              |
| 2:1:2988:A:H2'       | 2:1:2989:A:C8        | 2.51                     | 0.46              |
| 5:4:5:U:H2'          | 5:4:6:U:H6           | 1.80                     | 0.46              |
| 10:A:1235:U:O2'      | 42:g:177:MET:HE2     | 2.16                     | 0.46              |
| 10:A:1520:C:OP2      | 36:a:77:ARG:NH2      | 2.48                     | 0.46              |
| 10:A:1584:A:C8       | 40:e:14:PHE:HD2      | 2.32                     | 0.46              |
| 18:I:63:LEU:O        | 18:I:67:ARG:HG2      | 2.15                     | 0.46              |
| 33:X:71:LYS:HB3      | 33:X:130:TYR:CZ      | 2.49                     | 0.46              |
| 39:d:12:VAL:HG22     | 39:d:30:VAL:HG12     | 1.98                     | 0.46              |
| 43:h:42:LEU:HD23     | 43:h:42:LEU:H        | 1.81                     | 0.46              |
| 43:h:192:HIS:HB3     | 43:h:214:ASP:OD2     | 2.16                     | 0.46              |
| 57:w:9:VAL:HG12      | 57:w:118:ARG:HG3     | 1.96                     | 0.46              |
| 2:1:422:A:C2         | 2:1:2341:A:H4'       | 2.50                     | 0.46              |
| 2:1:685:U:OP2        | 54:t:36:ARG:NH2      | 2.40                     | 0.46              |
| 2:1:788:G:H2'        | 2:1:789:C:C6         | 2.50                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:1:981:U:H2'     | 2:1:982:U:H6      | 1.81                     | 0.46              |
| 2:1:1817:U:O4     | 68:AH:67:LYS:NZ   | 2.46                     | 0.46              |
| 2:1:2385:C:H2'    | 2:1:2386:U:H6     | 1.80                     | 0.46              |
| 2:1:2488:U:O2'    | 2:1:2489:A:H8     | 1.99                     | 0.46              |
| 10:A:68:A:C6      | 17:H:132:ARG:HD2  | 2.51                     | 0.46              |
| 10:A:641:G:H2'    | 10:A:642:C:H6     | 1.80                     | 0.46              |
| 10:A:886:G:H2'    | 10:A:887:G:C8     | 2.50                     | 0.46              |
| 10:A:1052:G:H5''  | 12:C:150:ILE:HG12 | 1.98                     | 0.46              |
| 10:A:1763:A:OP2   | 75:AO:11:ARG:NH2  | 2.49                     | 0.46              |
| 15:F:15:PRO:HG2   | 15:F:18:TRP:CE2   | 2.51                     | 0.46              |
| 15:F:103:TYR:HE2  | 15:F:184:THR:HG23 | 1.78                     | 0.46              |
| 17:H:118:ASP:OD1  | 17:H:119:ASN:N    | 2.49                     | 0.46              |
| 28:R:139:LYS:HE2  | 28:R:141:TYR:HE1  | 1.80                     | 0.46              |
| 35:Z:74:LEU:HD12  | 35:Z:90:ARG:NH2   | 2.28                     | 0.46              |
| 64:AD:88:ARG:CZ   | 77:AQ:44:LYS:HG2  | 2.46                     | 0.46              |
| 1:0:64:ILE:HG12   | 46:l:360:VAL:HG22 | 1.98                     | 0.46              |
| 1:0:66:GLU:HG2    | 1:0:98:THR:HG22   | 1.98                     | 0.46              |
| 2:1:493:A:O2'     | 2:1:3238:A:N1     | 2.45                     | 0.46              |
| 2:1:963:A:OP1     | 62:AB:47:LYS:NZ   | 2.45                     | 0.46              |
| 2:1:1474:C:H2'    | 2:1:1475:U:C6     | 2.51                     | 0.46              |
| 2:1:1747:G:H5'    | 72:AL:26:LYS:HE2  | 1.98                     | 0.46              |
| 2:1:2855:U:H2'    | 2:1:2856:C:C6     | 2.51                     | 0.46              |
| 4:3:110:G:P       | 47:m:279:ARG:HD3  | 2.56                     | 0.46              |
| 10:A:846:U:O2'    | 33:X:56:HIS:O     | 2.34                     | 0.46              |
| 10:A:1338:U:C2    | 10:A:1339:G:C8    | 3.04                     | 0.46              |
| 10:A:1783:C:O2    | 37:b:92:ARG:HB3   | 2.16                     | 0.46              |
| 37:b:88:SER:O     | 37:b:92:ARG:HG3   | 2.16                     | 0.46              |
| 53:s:160:ILE:HG22 | 53:s:164:LYS:HE2  | 1.97                     | 0.46              |
| 2:1:397:A:H5'     | 2:1:399:A:OP1     | 2.16                     | 0.46              |
| 2:1:1761:U:H2'    | 2:1:1762:G:H4'    | 1.97                     | 0.46              |
| 2:1:1948:G:H2'    | 2:1:2070:A:H61    | 1.80                     | 0.46              |
| 10:A:899:G:H5''   | 10:A:900:A:OP1    | 2.16                     | 0.46              |
| 10:A:912:C:O2'    | 25:P:119:IAS:OD1  | 2.34                     | 0.46              |
| 10:A:974:U:H2'    | 10:A:975:C:C6     | 2.51                     | 0.46              |
| 10:A:1545:U:H5''  | 10:A:1546:G:H4'   | 1.98                     | 0.46              |
| 10:A:1668:A:C8    | 17:H:65:GLN:HG3   | 2.51                     | 0.46              |
| 10:A:1675:U:H2'   | 10:A:1676:A:N3    | 2.31                     | 0.46              |
| 23:N:43:ARG:HH12  | 23:N:103:LEU:N    | 2.00                     | 0.46              |
| 28:R:54:VAL:O     | 28:R:58:LYS:NZ    | 2.34                     | 0.46              |
| 36:a:64:VAL:HG13  | 36:a:68:ARG:NH1   | 2.31                     | 0.46              |
| 43:h:202:SER:HG   | 43:h:206:SER:H    | 1.64                     | 0.46              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 55:u:121:ARG:O   | 55:u:125:LYS:HG2  | 2.16                     | 0.46              |
| 58:x:128:ARG:HD2 | 58:x:136:ILE:HG21 | 1.98                     | 0.46              |
| 2:1:374:A:N3     | 2:1:376:G:H5''    | 2.31                     | 0.46              |
| 2:1:983:U:H2'    | 2:1:984:U:C6      | 2.51                     | 0.46              |
| 2:1:2138:G:H2'   | 2:1:2139:G:C8     | 2.50                     | 0.46              |
| 2:1:2824:C:N3    | 52:r:158:LYS:HE3  | 2.30                     | 0.46              |
| 2:1:3005:A:H2'   | 2:1:3006:C:H6     | 1.81                     | 0.46              |
| 2:1:3139:U:H2'   | 2:1:3140:U:C6     | 2.51                     | 0.46              |
| 8:8:99:VAL:HG11  | 8:8:124:ILE:HD13  | 1.98                     | 0.46              |
| 10:A:68:A:C5     | 17:H:160:ARG:NH1  | 2.84                     | 0.46              |
| 10:A:1226:G:H4'  | 26:Q:78:THR:HA    | 1.98                     | 0.46              |
| 10:A:1478:A:H1'  | 10:A:1480:G:C4    | 2.50                     | 0.46              |
| 10:A:1562:G:H2'  | 10:A:1563:A:C8    | 2.51                     | 0.46              |
| 16:G:73:THR:N    | 16:G:91:GLU:OE2   | 2.45                     | 0.46              |
| 16:G:173:ALA:O   | 16:G:177:ILE:HG12 | 2.15                     | 0.46              |
| 36:a:65:LEU:HD13 | 36:a:80:LEU:HD11  | 1.96                     | 0.46              |
| 40:e:33:LYS:HE2  | 40:e:34:TYR:CZ    | 2.50                     | 0.46              |
| 78:PT:67:C:H2'   | 78:PT:68:C:C6     | 2.51                     | 0.46              |
| 2:1:74:G:H5'     | 54:t:58:VAL:HB    | 1.98                     | 0.46              |
| 2:1:1079:G:H2'   | 2:1:1080:A:C8     | 2.51                     | 0.46              |
| 2:1:1284:U:H2'   | 2:1:1285:G:H8     | 1.81                     | 0.46              |
| 2:1:2330:A:H5''  | 58:x:83:TRP:O     | 2.16                     | 0.46              |
| 10:A:261:C:O2'   | 10:A:262:G:H5'    | 2.16                     | 0.46              |
| 10:A:290:U:H2'   | 10:A:291:U:C6     | 2.51                     | 0.46              |
| 10:A:471:A:H2'   | 10:A:472:A:O4'    | 2.15                     | 0.46              |
| 10:A:1002:U:H2'  | 10:A:1003:U:C6    | 2.50                     | 0.46              |
| 10:A:1571:G:O4'  | 28:R:121:ARG:NH2  | 2.49                     | 0.46              |
| 13:D:135:ARG:HB2 | 13:D:217:TYR:CD1  | 2.51                     | 0.46              |
| 21:L:39:ASN:O    | 21:L:43:ILE:HG12  | 2.16                     | 0.46              |
| 23:N:24:ILE:HB   | 23:N:28:LEU:HD21  | 1.97                     | 0.46              |
| 29:S:24:LEU:CB   | 29:S:58:MET:HE3   | 2.46                     | 0.46              |
| 61:AA:22:LYS:NZ  | 61:AA:129:TRP:O   | 2.46                     | 0.46              |
| 78:AT:65:G:C4    | 78:AT:66:C:C5     | 3.04                     | 0.46              |
| 2:1:730:A:H4'    | 2:1:730:A:OP1     | 2.15                     | 0.45              |
| 2:1:1050:A:H5''  | 2:1:2609:A:H61    | 1.80                     | 0.45              |
| 2:1:1764:C:H2'   | 2:1:1765:G:H8     | 1.81                     | 0.45              |
| 5:4:10:A:H2'     | 5:4:11:C:C6       | 2.50                     | 0.45              |
| 10:A:15:U:H2'    | 10:A:16:G:O4'     | 2.16                     | 0.45              |
| 10:A:569:G:H4'   | 34:Y:114:LYS:HD2  | 1.98                     | 0.45              |
| 10:A:803:G:C6    | 10:A:838:G:C6     | 3.04                     | 0.45              |
| 10:A:1674:U:H2'  | 10:A:1675:U:C6    | 2.51                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:B:118:PRO:HG2  | 11:B:141:ILE:HD13 | 1.98                     | 0.45              |
| 14:E:41:ARG:HB2   | 14:E:48:GLU:HB2   | 1.98                     | 0.45              |
| 31:V:43:ASN:O     | 31:V:46:GLN:HG2   | 2.15                     | 0.45              |
| 44:j:207:VAL:HG23 | 44:j:208:ASP:OD1  | 2.17                     | 0.45              |
| 47:m:260:PHE:HB3  | 47:m:264:GLN:HB2  | 1.98                     | 0.45              |
| 54:t:62:THR:CG2   | 62:AB:66:ASN:HB3  | 2.46                     | 0.45              |
| 2:1:169:G:O6      | 2:1:249:G:H1'     | 2.16                     | 0.45              |
| 2:1:1563:A:H2'    | 2:1:1564:U:C6     | 2.50                     | 0.45              |
| 2:1:2407:G:H2'    | 2:1:2408:A:H8     | 1.81                     | 0.45              |
| 2:1:2908:A:OP2    | 81:1:3408:GET:N32 | 2.49                     | 0.45              |
| 10:A:21:U:O2'     | 20:K:16:LYS:O     | 2.33                     | 0.45              |
| 10:A:154:A:H2'    | 10:A:155:A:O4'    | 2.16                     | 0.45              |
| 10:A:940:A:H4'    | 10:A:1058:G:O2'   | 2.15                     | 0.45              |
| 10:A:1035:G:OP1   | 38:c:70:LYS:NZ    | 2.37                     | 0.45              |
| 26:Q:64:ARG:HD3   | 26:Q:92:SER:HB2   | 1.98                     | 0.45              |
| 28:R:4:GLN:HB2    | 28:R:23:ALA:HB2   | 1.98                     | 0.45              |
| 28:R:58:LYS:HB3   | 28:R:88:LEU:HD11  | 1.98                     | 0.45              |
| 32:W:74:GLN:HB2   | 32:W:79:LEU:HB3   | 1.98                     | 0.45              |
| 53:s:65:ILE:HG13  | 53:s:66:ALA:N     | 2.31                     | 0.45              |
| 62:AB:36:GLY:HA3  | 62:AB:40:HIS:CE1  | 2.51                     | 0.45              |
| 78:AT:17:C:OP2    | 78:AT:18(A):U:O2' | 2.33                     | 0.45              |
| 2:1:1069:U:H2'    | 2:1:1070:U:C6     | 2.51                     | 0.45              |
| 2:1:2656:C:O2'    | 53:s:99:THR:HG21  | 2.15                     | 0.45              |
| 4:3:113:C:H2'     | 4:3:114:U:O4'     | 2.16                     | 0.45              |
| 10:A:415:A:H5'    | 10:A:416:G:C4     | 2.52                     | 0.45              |
| 10:A:1154:G:N1    | 10:A:1562:G:OP2   | 2.38                     | 0.45              |
| 18:I:67:ARG:HD2   | 18:I:127:PHE:CE1  | 2.51                     | 0.45              |
| 19:J:4:SER:HB2    | 19:J:24:LYS:HD3   | 1.97                     | 0.45              |
| 27:T:49:LYS:HG3   | 27:T:81:ILE:HD11  | 1.98                     | 0.45              |
| 28:R:12:LYS:O     | 28:R:13:LYS:C     | 2.59                     | 0.45              |
| 45:k:217:VAL:HG11 | 45:k:328:ILE:HD12 | 1.97                     | 0.45              |
| 47:m:91:GLY:O     | 47:m:94:ASN:ND2   | 2.49                     | 0.45              |
| 54:t:62:THR:O     | 54:t:65:TYR:N     | 2.35                     | 0.45              |
| 1:0:82:GLU:OE1    | 4:3:95:A:H4'      | 2.17                     | 0.45              |
| 2:1:2107:U:H2'    | 2:1:2108:G:C8     | 2.51                     | 0.45              |
| 2:1:2587:G:H2'    | 2:1:2588:C:H6     | 1.80                     | 0.45              |
| 16:G:117:ALA:O    | 16:G:120:ILE:HG22 | 2.17                     | 0.45              |
| 16:G:147:THR:HG23 | 39:d:45:LYS:NZ    | 2.31                     | 0.45              |
| 23:N:50:LYS:HZ2   | 42:g:144:VAL:HG22 | 1.82                     | 0.45              |
| 34:Y:126:LYS:HG2  | 34:Y:131:SER:HA   | 1.99                     | 0.45              |
| 43:h:110:ASP:HB2  | 43:h:128:ARG:HD3  | 1.98                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 53:s:13:ARG:HH12  | 53:s:15:GLU:HG2   | 1.81                     | 0.45              |
| 64:AD:11:ASN:O    | 64:AD:14:SER:OG   | 2.29                     | 0.45              |
| 78:PT:64:G:H2'    | 78:PT:65:G:C8     | 2.50                     | 0.45              |
| 2:1:922:A:H2'     | 2:1:923:C:C6      | 2.52                     | 0.45              |
| 5:4:90:U:O2'      | 5:4:92:A:OP1      | 2.30                     | 0.45              |
| 10:A:504:A:HO2'   | 10:A:505:U:P      | 2.39                     | 0.45              |
| 10:A:720:C:H1'    | 10:A:721:C:C5     | 2.52                     | 0.45              |
| 10:A:1235:U:H2'   | 10:A:1236:U:C2    | 2.51                     | 0.45              |
| 10:A:1246:G:H2'   | 10:A:1247:U:H6    | 1.82                     | 0.45              |
| 10:A:1452:G:O2'   | 10:A:1589:C:OP1   | 2.33                     | 0.45              |
| 13:D:35:LYS:HB3   | 13:D:242:ALA:HB1  | 1.97                     | 0.45              |
| 29:S:109:LEU:O    | 29:S:112:SER:OG   | 2.31                     | 0.45              |
| 31:V:49:ILE:HG23  | 31:V:94:ALA:HB2   | 1.99                     | 0.45              |
| 2:1:405:U:O4      | 81:1:3403:GET:O61 | 2.15                     | 0.45              |
| 2:1:2191:A:H2'    | 2:1:2192:A:H8     | 1.80                     | 0.45              |
| 2:1:2201:A:H2'    | 2:1:2202:A:C8     | 2.52                     | 0.45              |
| 5:4:2:A:C4        | 5:4:3:A:C8        | 3.05                     | 0.45              |
| 5:4:19:C:H2'      | 5:4:20:U:C6       | 2.52                     | 0.45              |
| 10:A:249:A:C2     | 15:F:131:LEU:HD12 | 2.51                     | 0.45              |
| 11:B:18:LEU:HD23  | 29:S:100:LEU:HG   | 1.98                     | 0.45              |
| 13:D:96:VAL:HG21  | 13:D:203:GLU:HG3  | 1.98                     | 0.45              |
| 14:E:138:VAL:HG22 | 14:E:152:LYS:HG2  | 1.98                     | 0.45              |
| 16:G:99:MET:O     | 16:G:103:ASN:HB2  | 2.17                     | 0.45              |
| 18:I:74:THR:O     | 18:I:78:GLU:HG2   | 2.16                     | 0.45              |
| 39:d:30:VAL:HG22  | 39:d:40:ILE:O     | 2.17                     | 0.45              |
| 48:n:55:LYS:NZ    | 48:n:100:PHE:O    | 2.37                     | 0.45              |
| 57:w:77:PRO:HB3   | 57:w:139:VAL:HG12 | 1.98                     | 0.45              |
| 2:1:247:C:H2'     | 2:1:248:U:C6      | 2.51                     | 0.45              |
| 2:1:546:C:H2'     | 2:1:547:U:O4'     | 2.17                     | 0.45              |
| 2:1:3135:A:H61    | 2:1:3250:C:H42    | 1.63                     | 0.45              |
| 2:1:3154:A:N3     | 2:1:3157:A:O2'    | 2.47                     | 0.45              |
| 10:A:52:U:H2'     | 10:A:53:G:C8      | 2.52                     | 0.45              |
| 10:A:193:G:C2     | 10:A:194:G:C5     | 3.05                     | 0.45              |
| 10:A:364:A:OP1    | 10:A:743:U:O2'    | 2.28                     | 0.45              |
| 10:A:1012:A:OP1   | 10:A:1776:G:O2'   | 2.24                     | 0.45              |
| 10:A:1213:G:H22   | 23:N:67:THR:HG23  | 1.82                     | 0.45              |
| 10:A:1663:U:H2'   | 10:A:1664:C:C6    | 2.51                     | 0.45              |
| 14:E:12:LEU:HD22  | 31:V:85:ILE:HG12  | 1.98                     | 0.45              |
| 28:R:26:GLY:HA2   | 28:R:59:PHE:O     | 2.17                     | 0.45              |
| 29:S:56:HIS:CE1   | 29:S:60:ARG:HD3   | 2.52                     | 0.45              |
| 39:d:34:GLU:OE1   | 39:d:34:GLU:N     | 2.50                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 42:g:182:TYR:HD1  | 42:g:189:THR:HB   | 1.81                     | 0.45              |
| 45:k:256:HIS:HA   | 45:k:257:PRO:C    | 2.40                     | 0.45              |
| 48:n:95:VAL:HG12  | 48:n:97:VAL:HG13  | 1.98                     | 0.45              |
| 72:AL:5:ILE:O     | 72:AL:54:LEU:HD12 | 2.17                     | 0.45              |
| 2:1:843:A:H2'     | 2:1:844:A:C8      | 2.52                     | 0.45              |
| 2:1:1715:G:N7     | 60:z:121:HIS:HE1  | 2.14                     | 0.45              |
| 2:1:3324:A:H2'    | 2:1:3325:C:C6     | 2.52                     | 0.45              |
| 10:A:142:G:H1     | 10:A:169:A:H61    | 1.64                     | 0.45              |
| 10:A:871:U:C2     | 10:A:872:A:C8     | 3.05                     | 0.45              |
| 10:A:1188:A:C2    | 10:A:1543:A:C4    | 3.05                     | 0.45              |
| 10:A:1341:U:O2    | 10:A:1352:G:N2    | 2.36                     | 0.45              |
| 10:A:1437:C:OP1   | 40:e:12:ARG:NH1   | 2.41                     | 0.45              |
| 11:B:142:PRO:HG3  | 32:W:32:VAL:HB    | 1.99                     | 0.45              |
| 15:F:181:VAL:HG12 | 15:F:227:VAL:HA   | 1.98                     | 0.45              |
| 16:G:123:VAL:HG11 | 36:a:59:TYR:HD1   | 1.82                     | 0.45              |
| 17:H:102:VAL:HG13 | 17:H:106:LEU:HD12 | 1.98                     | 0.45              |
| 18:I:108:ARG:HD2  | 18:I:109:PRO:O    | 2.17                     | 0.45              |
| 28:R:6:VAL:HG22   | 28:R:21:VAL:HB    | 1.99                     | 0.45              |
| 46:l:111:ASN:ND2  | 56:v:201:ARG:HB3  | 2.20                     | 0.45              |
| 47:m:55:PHE:CE2   | 47:m:60:ILE:HG12  | 2.52                     | 0.45              |
| 61:AA:81:MET:HE3  | 61:AA:82:PRO:HD2  | 1.99                     | 0.45              |
| 67:AG:8:TYR:CE1   | 67:AG:99:ARG:HG2  | 2.52                     | 0.45              |
| 2:1:502:U:H2'     | 2:1:503:U:C6      | 2.52                     | 0.45              |
| 2:1:1569:C:H3'    | 2:1:1570:A:H8     | 1.82                     | 0.45              |
| 2:1:2519:A:H4'    | 2:1:2520:A:O5'    | 2.16                     | 0.45              |
| 2:1:2978:A:H2'    | 2:1:2979:U:O4'    | 2.16                     | 0.45              |
| 9:9:48:LEU:HD13   | 9:9:115:ARG:HH21  | 1.82                     | 0.45              |
| 10:A:683:G:H2'    | 10:A:684:C:H6     | 1.81                     | 0.45              |
| 10:A:727:U:H1'    | 18:I:103:ARG:NH1  | 2.31                     | 0.45              |
| 10:A:1702:A:H2'   | 10:A:1703:C:H5'   | 1.99                     | 0.45              |
| 11:B:24:LEU:HD12  | 11:B:41:ARG:NH2   | 2.31                     | 0.45              |
| 21:L:13:GLN:OE1   | 21:L:80:LEU:HD13  | 2.17                     | 0.45              |
| 27:T:42:TYR:CZ    | 27:T:99:HIS:CD2   | 3.05                     | 0.45              |
| 28:R:93:GLN:O     | 43:h:60:LYS:HE3   | 2.17                     | 0.45              |
| 30:U:106:GLN:O    | 30:U:109:GLN:HB2  | 2.17                     | 0.45              |
| 33:X:23:ARG:HD3   | 33:X:65:LEU:O     | 2.16                     | 0.45              |
| 52:r:187:ASN:OD1  | 52:r:217:GLN:HB2  | 2.17                     | 0.45              |
| 52:r:200:LEU:N    | 52:r:213:PHE:HE2  | 2.14                     | 0.45              |
| 53:s:166:ARG:HD2  | 53:s:167:TYR:CE1  | 2.51                     | 0.45              |
| 78:PT:50:G:H2'    | 78:PT:51:U:C6     | 2.52                     | 0.45              |
| 2:1:357:A:O4'     | 46:l:82:GLY:HA3   | 2.17                     | 0.45              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 2:1:407:A:C2       | 5:4:17:A:H1'      | 2.52                     | 0.45              |
| 2:1:2988:A:H2'     | 2:1:2989:A:H8     | 1.81                     | 0.45              |
| 3:2:80:VAL:HB      | 3:2:83:ARG:HH12   | 1.81                     | 0.45              |
| 10:A:74:U:O2'      | 10:A:75:U:H3'     | 2.17                     | 0.45              |
| 10:A:442:C:H5      | 35:Z:105:ARG:HH22 | 1.63                     | 0.45              |
| 10:A:932:U:H2'     | 10:A:933:A:H8     | 1.82                     | 0.45              |
| 10:A:1394:G:O3'    | 43:h:17:ASN:ND2   | 2.46                     | 0.45              |
| 10:A:1629:G:N7     | 81:A:1801:GET:N33 | 2.63                     | 0.45              |
| 15:F:22:LYS:HB3    | 15:F:23:LEU:HD12  | 1.99                     | 0.45              |
| 28:R:72:GLY:N      | 28:R:75:SER:OG    | 2.31                     | 0.45              |
| 45:k:68:HIS:CD2    | 45:k:69:LYS:HE2   | 2.52                     | 0.45              |
| 52:r:38:ARG:HG2    | 52:r:41:ALA:HB2   | 1.99                     | 0.45              |
| 54:t:48:PRO:HD2    | 69:AI:115:LYS:HE2 | 1.99                     | 0.45              |
| 71:AK:64:MET:O     | 71:AK:68:LYS:HB2  | 2.17                     | 0.45              |
| 1:0:95:ARG:HG2     | 1:0:95:ARG:HH11   | 1.81                     | 0.44              |
| 2:1:848:U:C6       | 77:AQ:2:THR:HG22  | 2.53                     | 0.44              |
| 2:1:1895:G:O2'     | 2:1:2312:U:O4     | 2.27                     | 0.44              |
| 2:1:2587:G:H2'     | 2:1:2588:C:C6     | 2.53                     | 0.44              |
| 2:1:3139:U:H2'     | 2:1:3140:U:H6     | 1.82                     | 0.44              |
| 81:1:3408:GET:H833 | 45:k:6:TYR:OH     | 2.17                     | 0.44              |
| 10:A:119:A:H1'     | 10:A:395:A:C5     | 2.51                     | 0.44              |
| 10:A:524:A:OP2     | 35:Z:93:ARG:NH2   | 2.38                     | 0.44              |
| 10:A:881:U:H2'     | 10:A:882:C:C6     | 2.52                     | 0.44              |
| 10:A:1327:C:H4'    | 43:h:103:ARG:HH21 | 1.82                     | 0.44              |
| 13:D:225:TRP:CG    | 33:X:68:ARG:HD3   | 2.52                     | 0.44              |
| 16:G:63:GLN:OE1    | 16:G:66:ASN:HB2   | 2.17                     | 0.44              |
| 18:I:81:PHE:HB3    | 18:I:84:ARG:CZ    | 2.47                     | 0.44              |
| 45:k:21:ARG:HE     | 45:k:269:GLN:HG3  | 1.81                     | 0.44              |
| 56:v:51:LEU:HD22   | 56:v:117:ASN:ND2  | 2.32                     | 0.44              |
| 58:x:27:LYS:HE2    | 58:x:63:TYR:CD1   | 2.52                     | 0.44              |
| 78:PT:56:U:O2'     | 78:PT:58:A:N7     | 2.48                     | 0.44              |
| 1:0:171:PHE:O      | 1:0:172:TYR:HB2   | 2.17                     | 0.44              |
| 2:1:211:G:H2'      | 46:l:222:ASN:OD1  | 2.16                     | 0.44              |
| 2:1:527:G:H2'      | 2:1:528:A:C8      | 2.52                     | 0.44              |
| 2:1:912:G:H5'      | 2:1:913:A:OP1     | 2.17                     | 0.44              |
| 4:3:55:A:P         | 53:s:3:ASP:H      | 2.40                     | 0.44              |
| 10:A:218:A:OP2     | 10:A:816:U:O2'    | 2.29                     | 0.44              |
| 10:A:329:A:H5'     | 19:J:33:PRO:HA    | 1.99                     | 0.44              |
| 10:A:870:G:H2'     | 10:A:871:U:C6     | 2.53                     | 0.44              |
| 10:A:902:U:O2      | 25:P:36:ARG:NH1   | 2.49                     | 0.44              |
| 10:A:1239:U:OP2    | 23:N:46:ARG:NH1   | 2.49                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:B:92:HIS:O      | 11:B:182:LEU:HD21  | 2.17                     | 0.44              |
| 12:C:30:PHE:HD1    | 12:C:94:LYS:HA     | 1.82                     | 0.44              |
| 14:E:72:SER:HA     | 14:E:75:VAL:HG22   | 1.99                     | 0.44              |
| 36:a:50:ILE:O      | 36:a:54:VAL:HG22   | 2.16                     | 0.44              |
| 59:y:126:GLN:O     | 59:y:130:ARG:HG2   | 2.18                     | 0.44              |
| 2:1:30:C:H4'       | 56:v:96:LYS:HE2    | 1.99                     | 0.44              |
| 2:1:587:A:H8       | 2:1:588:G:C8       | 2.35                     | 0.44              |
| 2:1:708:A:H2'      | 2:1:709:A:C8       | 2.51                     | 0.44              |
| 2:1:988:A:O2'      | 2:1:989:G:H5'      | 2.17                     | 0.44              |
| 4:3:3:U:H2'        | 4:3:4:U:H6         | 1.81                     | 0.44              |
| 10:A:129:A:N1      | 10:A:179:A:N6      | 2.66                     | 0.44              |
| 10:A:1279:G:O2'    | 10:A:1306:A:N1     | 2.50                     | 0.44              |
| 19:J:199:LEU:O     | 19:J:203:THR:HG23  | 2.18                     | 0.44              |
| 27:T:8:GLN:HB3     | 36:a:44:GLN:HG2    | 2.00                     | 0.44              |
| 35:Z:15:ASN:HD21   | 35:Z:18:LEU:HD12   | 1.83                     | 0.44              |
| 43:h:166:VAL:N     | 43:h:178:TRP:O     | 2.42                     | 0.44              |
| 45:k:117:ARG:HA    | 45:k:117:ARG:HD2   | 1.84                     | 0.44              |
| 48:n:42:LEU:HD21   | 48:n:84:ILE:HG13   | 1.98                     | 0.44              |
| 70:AJ:86:VAL:O     | 70:AJ:90:THR:HG23  | 2.18                     | 0.44              |
| 78:AT:59:A:O2'     | 78:AT:61:U:OP2     | 2.26                     | 0.44              |
| 2:1:258:U:H2'      | 2:1:259:C:C6       | 2.52                     | 0.44              |
| 2:1:3297:U:OP1     | 7:7:35:LYS:HD3     | 2.16                     | 0.44              |
| 81:1:3404:GET:H712 | 81:1:3404:GET:H322 | 1.82                     | 0.44              |
| 10:A:1067:C:H5''   | 10:A:1068:G:H8     | 1.83                     | 0.44              |
| 10:A:1226:G:C4     | 26:Q:79:HIS:CD2    | 3.06                     | 0.44              |
| 10:A:1398:G:H4'    | 10:A:1399:U:O5'    | 2.17                     | 0.44              |
| 14:E:7:SER:O       | 14:E:11:LYS:N      | 2.36                     | 0.44              |
| 21:L:56:LYS:HE3    | 21:L:67:THR:HB     | 2.00                     | 0.44              |
| 24:O:66:VAL:HG23   | 24:O:67:THR:HG23   | 1.99                     | 0.44              |
| 28:R:27:LEU:HD11   | 28:R:29:LYS:HD3    | 1.99                     | 0.44              |
| 28:R:53:LEU:HD23   | 28:R:107:ILE:HG22  | 1.99                     | 0.44              |
| 42:g:144:VAL:HG13  | 42:g:148:TYR:CE1   | 2.53                     | 0.44              |
| 43:h:38:ARG:HB3    | 43:h:68:ILE:HG12   | 1.99                     | 0.44              |
| 51:q:50:ASN:OD1    | 55:u:2:SER:HA      | 2.18                     | 0.44              |
| 53:s:28:ASP:CG     | 53:s:32:ARG:HH21   | 2.25                     | 0.44              |
| 53:s:125:MET:SD    | 53:s:127:PHE:HE1   | 2.41                     | 0.44              |
| 2:1:1093:G:H8      | 3:2:112:ASN:HD21   | 1.64                     | 0.44              |
| 2:1:1124:U:H2'     | 2:1:1125:A:O4'     | 2.17                     | 0.44              |
| 2:1:2182:C:H2'     | 2:1:2183:U:C6      | 2.52                     | 0.44              |
| 2:1:2632:G:OP1     | 2:1:2722:U:O2'     | 2.29                     | 0.44              |
| 2:1:3162:U:H2'     | 2:1:3163:U:O4'     | 2.17                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:1:3249:G:H2'    | 2:1:3250:C:C6     | 2.53                     | 0.44              |
| 6:6:135:VAL:HG11  | 7:7:26:SER:CB     | 2.46                     | 0.44              |
| 10:A:1092:G:O2'   | 10:A:1093:G:H5'   | 2.16                     | 0.44              |
| 15:F:192:VAL:HG21 | 15:F:239:LEU:HD11 | 2.00                     | 0.44              |
| 17:H:115:LYS:HB3  | 17:H:115:LYS:HE2  | 1.83                     | 0.44              |
| 18:I:135:ARG:HD2  | 33:X:51:GLU:OE2   | 2.18                     | 0.44              |
| 26:Q:52:LYS:HE2   | 26:Q:80:LEU:HD13  | 1.98                     | 0.44              |
| 28:R:72:GLY:H     | 28:R:75:SER:HG    | 1.60                     | 0.44              |
| 45:k:188:VAL:O    | 45:k:192:VAL:HG23 | 2.18                     | 0.44              |
| 48:n:130:ILE:HG23 | 48:n:134:ARG:HD2  | 1.99                     | 0.44              |
| 71:AK:52:LYS:HE2  | 71:AK:55:ARG:NH2  | 2.32                     | 0.44              |
| 2:1:673:C:O2'     | 2:1:677:U:OP1     | 2.27                     | 0.44              |
| 2:1:951:U:H2'     | 2:1:952:U:C6      | 2.52                     | 0.44              |
| 2:1:2386:U:H5'    | 63:AC:1:MET:SD    | 2.58                     | 0.44              |
| 10:A:213:A:N6     | 10:A:240:U:OP2    | 2.49                     | 0.44              |
| 10:A:1109:A:H2'   | 10:A:1110:A:C8    | 2.53                     | 0.44              |
| 10:A:1671:G:H2'   | 10:A:1672:G:O4'   | 2.17                     | 0.44              |
| 11:B:167:LYS:NZ   | 11:B:203:PHE:HB3  | 2.33                     | 0.44              |
| 13:D:171:LYS:HE2  | 13:D:192:TYR:CE1  | 2.53                     | 0.44              |
| 27:T:62:THR:OG1   | 27:T:65:GLU:OE1   | 2.28                     | 0.44              |
| 31:V:101:ARG:O    | 31:V:105:ILE:HG12 | 2.17                     | 0.44              |
| 47:m:153:THR:HG23 | 47:m:160:PHE:HZ   | 1.83                     | 0.44              |
| 55:u:46:GLN:O     | 55:u:48:GLN:NE2   | 2.40                     | 0.44              |
| 61:AA:116:LYS:O   | 61:AA:120:GLU:HG3 | 2.17                     | 0.44              |
| 72:AL:35:GLY:O    | 72:AL:36:LYS:HE2  | 2.17                     | 0.44              |
| 78:AT:17:C:H3'    | 78:AT:18(A):U:H2' | 1.99                     | 0.44              |
| 2:1:3061:C:H2'    | 2:1:3062:U:O4'    | 2.18                     | 0.44              |
| 2:1:3134:C:H2'    | 2:1:3135:A:C8     | 2.52                     | 0.44              |
| 10:A:93:A:H1'     | 15:F:3:ARG:HB3    | 1.99                     | 0.44              |
| 10:A:213:A:N6     | 10:A:240:U:H5''   | 2.32                     | 0.44              |
| 10:A:721:C:O2'    | 10:A:722:A:H8     | 2.00                     | 0.44              |
| 11:B:9:LEU:HD13   | 11:B:54:TRP:CG    | 2.53                     | 0.44              |
| 13:D:143:LEU:HD13 | 32:W:4:ASP:OD2    | 2.17                     | 0.44              |
| 23:N:69:GLU:OE1   | 23:N:69:GLU:N     | 2.51                     | 0.44              |
| 35:Z:6:THR:HB     | 35:Z:28:LEU:HB2   | 1.99                     | 0.44              |
| 43:h:211:ALA:HB3  | 43:h:240:LEU:HD13 | 2.00                     | 0.44              |
| 52:r:179:ASP:OD1  | 52:r:180:GLU:N    | 2.51                     | 0.44              |
| 2:1:18:U:H2'      | 2:1:19:A:C8       | 2.52                     | 0.44              |
| 2:1:1042:A:H2'    | 2:1:1045:C:C5     | 2.52                     | 0.44              |
| 2:1:2486:U:H2'    | 2:1:2487:U:C6     | 2.53                     | 0.44              |
| 2:1:3159:A:H2'    | 2:1:3160:C:H6     | 1.82                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:A:402:G:H2'    | 10:A:403:C:C6     | 2.53                     | 0.44              |
| 10:A:623:C:H2'    | 10:A:624:U:C6     | 2.53                     | 0.44              |
| 10:A:880:G:N2     | 25:P:33:THR:OG1   | 2.45                     | 0.44              |
| 10:A:1222:G:C2    | 10:A:1234:U:O4    | 2.71                     | 0.44              |
| 10:A:1473:A:H2'   | 10:A:1474:G:C8    | 2.52                     | 0.44              |
| 13:D:32:PRO:HD3   | 13:D:41:LYS:HZ1   | 1.83                     | 0.44              |
| 15:F:47:PHE:CE1   | 15:F:52:LEU:HD11  | 2.53                     | 0.44              |
| 15:F:124:GLY:HA2  | 15:F:142:HIS:CE1  | 2.52                     | 0.44              |
| 16:G:98:MET:SD    | 16:G:107:LYS:HG3  | 2.57                     | 0.44              |
| 18:I:54:LEU:O     | 18:I:86:VAL:HA    | 2.18                     | 0.44              |
| 43:h:40:LYS:O     | 43:h:65:HIS:HB2   | 2.17                     | 0.44              |
| 43:h:80:TYR:CD1   | 43:h:94:ASP:HA    | 2.45                     | 0.44              |
| 43:h:158:SER:HA   | 43:h:201:LEU:HD13 | 1.99                     | 0.44              |
| 45:k:283:TYR:CD1  | 45:k:354:VAL:HG21 | 2.52                     | 0.44              |
| 61:AA:41:ALA:HB2  | 61:AA:77:TYR:HE1  | 1.83                     | 0.44              |
| 68:AH:22:VAL:HG12 | 68:AH:30:LEU:HD11 | 2.00                     | 0.44              |
| 2:l:88:G:H21      | 2:l:281:G:H4'     | 1.83                     | 0.44              |
| 2:l:206:U:H2'     | 2:l:207:C:C6      | 2.53                     | 0.44              |
| 2:l:214:G:H5''    | 9:9:12:ARG:HG3    | 2.00                     | 0.44              |
| 2:l:1116:A:H2'    | 2:l:1117:U:H6     | 1.83                     | 0.44              |
| 2:l:2919:G:OP2    | 2:l:2919:G:H4'    | 2.17                     | 0.44              |
| 10:A:1:U:H5''     | 13:D:171:LYS:HZ2  | 1.83                     | 0.44              |
| 10:A:738:A:H2'    | 10:A:739:A:O4'    | 2.18                     | 0.44              |
| 10:A:1160:U:H2'   | 10:A:1161:G:H8    | 1.82                     | 0.44              |
| 10:A:1341:U:H2'   | 10:A:1342:A:H8    | 1.82                     | 0.44              |
| 19:J:190:LEU:HD22 | 19:J:194:GLU:HG2  | 2.00                     | 0.44              |
| 21:L:55:VAL:HG11  | 21:L:66:TYR:HB3   | 1.99                     | 0.44              |
| 36:a:84:GLU:HG2   | 36:a:91:PRO:HD3   | 2.00                     | 0.44              |
| 39:d:43:ASN:HD22  | 39:d:66:LEU:HD22  | 1.83                     | 0.44              |
| 44:j:209:HIS:HE1  | 44:j:211:HIS:CD2  | 2.25                     | 0.44              |
| 53:s:109:HIS:CD2  | 53:s:109:HIS:H    | 2.36                     | 0.44              |
| 59:y:151:ARG:O    | 59:y:161:LYS:HE3  | 2.18                     | 0.44              |
| 78:AT:73:A:H2'    | 78:AT:74:A:O4'    | 2.18                     | 0.44              |
| 1:0:172:TYR:OH    | 55:u:57:LEU:HG    | 2.18                     | 0.43              |
| 2:l:1591:U:C2     | 2:l:1592:C:C5     | 3.06                     | 0.43              |
| 2:l:1637:U:O2'    | 2:l:1638:A:H3'    | 2.17                     | 0.43              |
| 2:l:3197:G:H2'    | 2:l:3198:C:C6     | 2.52                     | 0.43              |
| 3:2:19:PHE:CE2    | 3:2:20:LYS:HE2    | 2.53                     | 0.43              |
| 9:9:86:GLN:HB3    | 9:9:94:SER:OG     | 2.18                     | 0.43              |
| 10:A:1039:U:H2'   | 10:A:1040:U:H6    | 1.82                     | 0.43              |
| 10:A:1476:A:H8    | 10:A:1501:A:H61   | 1.66                     | 0.43              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 10:A:1510:G:C8     | 30:U:79:LEU:HD13  | 2.53                     | 0.43              |
| 12:C:167:LYS:HA    | 12:C:170:GLU:HG2  | 1.99                     | 0.43              |
| 18:I:29:ASP:OD1    | 18:I:30:LEU:N     | 2.45                     | 0.43              |
| 28:R:98:GLU:HA     | 28:R:101:LYS:HG2  | 2.00                     | 0.43              |
| 45:k:292:ALA:HB1   | 45:k:295:ALA:HB3  | 2.00                     | 0.43              |
| 53:s:53:THR:HG23   | 53:s:60:ARG:HA    | 1.99                     | 0.43              |
| 53:s:108:GLU:CG    | 53:s:111:ASP:HB2  | 2.43                     | 0.43              |
| 56:v:159:ARG:HB2   | 56:v:164:LEU:HB2  | 1.99                     | 0.43              |
| 76:AP:104:LEU:HD23 | 76:AP:106:PHE:H   | 1.83                     | 0.43              |
| 2:1:117:U:O2       | 2:1:120:A:H5'     | 2.18                     | 0.43              |
| 2:1:385:A:H2'      | 2:1:386:A:C8      | 2.53                     | 0.43              |
| 3:2:102:ARG:O      | 3:2:106:LEU:HG    | 2.18                     | 0.43              |
| 5:4:6:U:H2'        | 5:4:7:U:C6        | 2.53                     | 0.43              |
| 9:9:51:ARG:HG2     | 9:9:52:GLN:N      | 2.34                     | 0.43              |
| 10:A:415:A:H5'     | 10:A:416:G:C5     | 2.52                     | 0.43              |
| 10:A:519:A:N3      | 35:Z:34:ASN:ND2   | 2.57                     | 0.43              |
| 10:A:1234:U:OP2    | 42:g:138:ARG:NH2  | 2.51                     | 0.43              |
| 10:A:1356:U:OP1    | 10:A:1356:U:H3'   | 2.18                     | 0.43              |
| 23:N:99:GLU:HB3    | 23:N:100:TRP:CE3  | 2.53                     | 0.43              |
| 39:d:11:LYS:HB2    | 39:d:53:ILE:HG12  | 1.99                     | 0.43              |
| 39:d:30:VAL:O      | 39:d:39:THR:HA    | 2.18                     | 0.43              |
| 46:l:139:ARG:NH2   | 46:l:241:PRO:HG2  | 2.26                     | 0.43              |
| 51:q:77:ASN:HA     | 51:q:80:THR:HG22  | 1.99                     | 0.43              |
| 53:s:30:LEU:HD13   | 53:s:65:ILE:O     | 2.18                     | 0.43              |
| 69:AI:8:GLU:O      | 69:AI:11:THR:OG1  | 2.36                     | 0.43              |
| 2:1:1626:U:O2'     | 2:1:1808:G:N2     | 2.44                     | 0.43              |
| 10:A:164:C:H4'     | 17:H:131:LYS:HE3  | 1.99                     | 0.43              |
| 10:A:510:A:H2'     | 10:A:511:U:O4'    | 2.18                     | 0.43              |
| 10:A:829:A:H2'     | 10:A:830:G:H8     | 1.83                     | 0.43              |
| 11:B:199:PRO:HB2   | 29:S:91:LEU:HD12  | 2.00                     | 0.43              |
| 15:F:141:THR:HG21  | 15:F:162:ILE:HD11 | 2.00                     | 0.43              |
| 25:P:58:ALA:O      | 25:P:62:VAL:HG23  | 2.18                     | 0.43              |
| 28:R:24:GLY:H      | 28:R:61:GLY:C     | 2.22                     | 0.43              |
| 28:R:142:ARG:NH1   | 78:PT:34:U:C5     | 2.87                     | 0.43              |
| 34:Y:92:CYS:HG     | 34:Y:136:TRP:CD1  | 2.36                     | 0.43              |
| 39:d:64:ARG:HG2    | 39:d:65:ARG:H     | 1.83                     | 0.43              |
| 43:h:88:ARG:HG2    | 43:h:109:GLY:C    | 2.44                     | 0.43              |
| 58:x:60:PHE:HB3    | 58:x:64:ASN:HB3   | 2.00                     | 0.43              |
| 64:AD:15:LYS:NZ    | 64:AD:105:SER:HB2 | 2.33                     | 0.43              |
| 68:AH:108:GLN:O    | 68:AH:112:GLU:HG2 | 2.18                     | 0.43              |
| 1:0:138[A]:GLN:HA  | 1:0:141:LYS:HB3   | 2.00                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:1:7:C:H2'       | 2:1:8:U:C6        | 2.53                     | 0.43              |
| 2:1:924:C:H2'     | 2:1:925:A:C8      | 2.53                     | 0.43              |
| 2:1:1345:G:H5''   | 2:1:1346:U:H5''   | 2.00                     | 0.43              |
| 2:1:1593:C:H2'    | 2:1:1594:G:C8     | 2.53                     | 0.43              |
| 2:1:1663:A:H2'    | 2:1:1664:G:H8     | 1.83                     | 0.43              |
| 2:1:2744:C:H1'    | 2:1:2745:C:H5     | 1.83                     | 0.43              |
| 7:7:20:LEU:HD13   | 7:7:30:ARG:HG2    | 2.01                     | 0.43              |
| 10:A:904:A:N3     | 25:P:31:LYS:NZ    | 2.56                     | 0.43              |
| 10:A:1026:G:H2'   | 10:A:1027:G:H8    | 1.77                     | 0.43              |
| 11:B:200:ASP:HA   | 11:B:203:PHE:CD2  | 2.53                     | 0.43              |
| 13:D:160:VAL:HG11 | 13:D:205:THR:HA   | 2.00                     | 0.43              |
| 14:E:139:ILE:HG22 | 14:E:143:LEU:HD21 | 2.00                     | 0.43              |
| 15:F:131:LEU:HA   | 15:F:137:PRO:HA   | 2.00                     | 0.43              |
| 17:H:135:PRO:HB2  | 17:H:141:ILE:HG13 | 2.00                     | 0.43              |
| 18:I:18:ALA:O     | 18:I:22:VAL:HG23  | 2.18                     | 0.43              |
| 19:J:145:VAL:HA   | 19:J:148:LYS:HG2  | 2.00                     | 0.43              |
| 28:R:24:GLY:HA3   | 28:R:63:ASP:HB2   | 2.01                     | 0.43              |
| 28:R:28:ILE:HA    | 28:R:64:ILE:HG12  | 2.00                     | 0.43              |
| 33:X:50:PHE:HB3   | 33:X:63:VAL:HG13  | 2.00                     | 0.43              |
| 76:AP:71:ARG:NH2  | 76:AP:80:LYS:HE2  | 2.33                     | 0.43              |
| 2:1:242:C:O2'     | 2:1:243:G:H5'     | 2.18                     | 0.43              |
| 6:6:13:MET:HE3    | 6:6:85:TRP:CE2    | 2.54                     | 0.43              |
| 10:A:861:G:H1'    | 10:A:929:A:O4'    | 2.18                     | 0.43              |
| 10:A:920:U:C4     | 37:b:15:ARG:NH1   | 2.82                     | 0.43              |
| 10:A:1143:C:O2'   | 10:A:1568:C:OP2   | 2.35                     | 0.43              |
| 10:A:1375:C:H6    | 29:S:28:PHE:CZ    | 2.36                     | 0.43              |
| 33:X:111:MET:HE2  | 33:X:111:MET:HB3  | 1.87                     | 0.43              |
| 40:e:30:LEU:HA    | 40:e:39:CYS:HA    | 2.00                     | 0.43              |
| 45:k:299:ASP:OD2  | 45:k:301:THR:HG22 | 2.19                     | 0.43              |
| 52:r:42:THR:HB    | 52:r:45:GLU:HG3   | 2.01                     | 0.43              |
| 58:x:178:SER:O    | 58:x:182:LEU:HG   | 2.19                     | 0.43              |
| 67:AG:8:TYR:CD1   | 67:AG:99:ARG:HG2  | 2.54                     | 0.43              |
| 78:AT:28:U:H2'    | 78:AT:29:C:H6     | 1.83                     | 0.43              |
| 2:1:19:A:H2'      | 2:1:20:G:C8       | 2.54                     | 0.43              |
| 2:1:1466:U:H2'    | 2:1:1467:U:C6     | 2.54                     | 0.43              |
| 2:1:1807:G:H2'    | 2:1:1808:G:O4'    | 2.19                     | 0.43              |
| 2:1:3044:C:H2'    | 2:1:3045:A:O4'    | 2.18                     | 0.43              |
| 3:2:69:LYS:HA     | 47:m:40:HIS:CE1   | 2.54                     | 0.43              |
| 4:3:70:A:H2'      | 4:3:71:U:C6       | 2.53                     | 0.43              |
| 10:A:152:G:H5'    | 17:H:108:VAL:HG11 | 2.01                     | 0.43              |
| 10:A:451:C:O2     | 10:A:451:C:H2'    | 2.19                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:A:537:G:OP2    | 10:A:537:G:N2     | 2.44                     | 0.43              |
| 21:L:9:LYS:O      | 21:L:13:GLN:HG2   | 2.19                     | 0.43              |
| 21:L:16:PHE:CD1   | 21:L:76:LEU:HD22  | 2.54                     | 0.43              |
| 21:L:31:LYS:NZ    | 21:L:36:ASP:OD1   | 2.41                     | 0.43              |
| 37:b:41:ILE:HD12  | 37:b:68:TYR:CD2   | 2.54                     | 0.43              |
| 39:d:32:PHE:HB2   | 39:d:35:ASP:O     | 2.18                     | 0.43              |
| 43:h:211:ALA:HB1  | 43:h:237:VAL:HG21 | 2.00                     | 0.43              |
| 46:l:359:GLU:OE2  | 49:o:73:TYR:OH    | 2.37                     | 0.43              |
| 47:m:211:LEU:HD23 | 47:m:219:TYR:HA   | 2.01                     | 0.43              |
| 2:1:1303:G:C4     | 57:w:61:LYS:HD3   | 2.54                     | 0.43              |
| 2:1:1720:U:OP2    | 60:z:128:LYS:NZ   | 2.45                     | 0.43              |
| 2:1:1761:U:H2'    | 2:1:1762:G:C4'    | 2.48                     | 0.43              |
| 2:1:2206:A:H2'    | 2:1:2207:A:C8     | 2.53                     | 0.43              |
| 2:1:2236:U:H2'    | 2:1:2237:A:O4'    | 2.19                     | 0.43              |
| 3:2:69:LYS:HG3    | 47:m:40:HIS:CD2   | 2.54                     | 0.43              |
| 10:A:786:G:H21    | 33:X:107:SER:HB3  | 1.84                     | 0.43              |
| 10:A:847:A:H5'    | 24:O:16:LEU:HD22  | 1.99                     | 0.43              |
| 10:A:1029:U:H2'   | 10:A:1030:C:C6    | 2.53                     | 0.43              |
| 10:A:1408:A:H2'   | 10:A:1409:U:C6    | 2.53                     | 0.43              |
| 10:A:1539:U:H2'   | 10:A:1540:G:C8    | 2.54                     | 0.43              |
| 10:A:1584:A:H8    | 40:e:14:PHE:HB2   | 1.82                     | 0.43              |
| 17:H:67:VAL:HB    | 17:H:99:GLY:HA2   | 2.00                     | 0.43              |
| 28:R:35:ILE:HG22  | 28:R:48:TYR:CE1   | 2.52                     | 0.43              |
| 31:V:44:ALA:HB1   | 31:V:49:ILE:HB    | 2.01                     | 0.43              |
| 43:h:252:ALA:HB2  | 43:h:289:LEU:HD13 | 2.00                     | 0.43              |
| 44:j:65:ASP:OD2   | 44:j:68:LYS:HG2   | 2.19                     | 0.43              |
| 56:v:114:ARG:HG2  | 56:v:137:PRO:HG3  | 2.00                     | 0.43              |
| 78:PT:3:C:H2'     | 78:PT:4:G:C8      | 2.54                     | 0.43              |
| 78:AT:11:A:H2'    | 78:AT:12:G:C8     | 2.53                     | 0.43              |
| 2:1:592:U:H2'     | 2:1:607:G:O6      | 2.19                     | 0.43              |
| 2:1:623:A:H2'     | 2:1:624:U:H6      | 1.84                     | 0.43              |
| 2:1:776:A:N7      | 59:y:178:ARG:NH1  | 2.65                     | 0.43              |
| 2:1:1387:C:C2     | 66:AF:104:ARG:HD3 | 2.53                     | 0.43              |
| 2:1:2537:U:OP1    | 50:p:33:LYS:NZ    | 2.49                     | 0.43              |
| 2:1:3174:G:O2'    | 55:u:99:LYS:HE2   | 2.18                     | 0.43              |
| 2:1:3208:A:OP1    | 57:w:160:LYS:NZ   | 2.44                     | 0.43              |
| 8:8:142:ILE:HD12  | 8:8:142:ILE:HA    | 1.84                     | 0.43              |
| 10:A:73:U:H4'     | 10:A:74:U:H5'     | 2.00                     | 0.43              |
| 10:A:592:A:OP2    | 20:K:37:LYS:HE3   | 2.19                     | 0.43              |
| 10:A:1516:C:H5'   | 28:R:41:GLU:OE2   | 2.18                     | 0.43              |
| 15:F:131:LEU:HD23 | 15:F:137:PRO:HB3  | 2.00                     | 0.43              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 16:G:25:LEU:HD22 | 28:R:26:GLY:HA3    | 2.00                     | 0.43              |
| 17:H:58:LYS:HG2  | 17:H:105:ASP:O     | 2.19                     | 0.43              |
| 33:X:36:LYS:O    | 33:X:40:VAL:HG23   | 2.19                     | 0.43              |
| 51:q:157:ASN:C   | 51:q:157:ASN:HD22  | 2.26                     | 0.43              |
| 53:s:108:GLU:HB2 | 53:s:110:ILE:HG12  | 2.00                     | 0.43              |
| 60:z:171:GLU:O   | 60:z:174:GLN:HB3   | 2.18                     | 0.43              |
| 2:1:268:A:C4     | 56:v:12:ARG:HG2    | 2.53                     | 0.43              |
| 2:1:417:A:H2'    | 2:1:418:A:C8       | 2.54                     | 0.43              |
| 2:1:762:U:H4'    | 2:1:763:U:O4'      | 2.18                     | 0.43              |
| 2:1:792:U:H2'    | 2:1:793:U:C6       | 2.54                     | 0.43              |
| 2:1:964:G:H2'    | 2:1:965:C:C6       | 2.54                     | 0.43              |
| 2:1:1347:U:O2    | 2:1:1347:U:H2'     | 2.18                     | 0.43              |
| 2:1:1641:U:O2'   | 2:1:1815:U:OP1     | 2.33                     | 0.43              |
| 2:1:2582:G:OP1   | 81:1:3412:GET:H531 | 2.18                     | 0.43              |
| 2:1:2919:G:C2    | 45:k:250:ALA:HB1   | 2.54                     | 0.43              |
| 4:3:3:U:H2'      | 4:3:4:U:C6         | 2.53                     | 0.43              |
| 10:A:138:C:N4    | 10:A:279:G:OP1     | 2.52                     | 0.43              |
| 10:A:207:U:H2'   | 10:A:208:A:H8      | 1.84                     | 0.43              |
| 10:A:1437:C:C2   | 10:A:1438:U:C5     | 3.06                     | 0.43              |
| 12:C:57:ALA:O    | 12:C:61:LEU:HD13   | 2.19                     | 0.43              |
| 12:C:108:ASP:OD1 | 12:C:109:LYS:N     | 2.51                     | 0.43              |
| 18:I:95:LEU:HD23 | 18:I:95:LEU:HA     | 1.91                     | 0.43              |
| 25:P:39:GLY:O    | 25:P:43:VAL:HG22   | 2.19                     | 0.43              |
| 27:T:64:GLU:HG2  | 27:T:65:GLU:N      | 2.34                     | 0.43              |
| 28:R:9:PHE:O     | 28:R:86:LYS:HD3    | 2.19                     | 0.43              |
| 28:R:49:GLU:O    | 28:R:53:LEU:HD13   | 2.18                     | 0.43              |
| 44:j:211:HIS:CE1 | 44:j:219:ILE:HG23  | 2.54                     | 0.43              |
| 49:o:39:ARG:HG2  | 49:o:39:ARG:HH11   | 1.84                     | 0.43              |
| 70:AJ:36:THR:O   | 70:AJ:40:ARG:HG3   | 2.19                     | 0.43              |
| 76:AP:37:ALA:O   | 76:AP:41:ARG:HG3   | 2.18                     | 0.43              |
| 2:1:561:U:H2'    | 2:1:562:C:C6       | 2.53                     | 0.43              |
| 2:1:1153:G:H2'   | 2:1:1154:A:O4'     | 2.19                     | 0.43              |
| 2:1:1560:U:O4    | 2:1:1571:G:O6      | 2.37                     | 0.43              |
| 6:6:74:MET:SD    | 6:6:102:ILE:HD13   | 2.59                     | 0.43              |
| 10:A:613:A:O2'   | 10:A:619:A:N1      | 2.47                     | 0.43              |
| 10:A:1118:A:H2'  | 10:A:1119:C:O4'    | 2.19                     | 0.43              |
| 10:A:1716:C:H2'  | 10:A:1717:A:O4'    | 2.18                     | 0.43              |
| 11:B:27:LYS:HA   | 11:B:45:MET:HA     | 2.01                     | 0.43              |
| 21:L:18:GLU:O    | 21:L:20:VAL:N      | 2.51                     | 0.43              |
| 23:N:26:ASP:O    | 23:N:28:LEU:N      | 2.52                     | 0.43              |
| 30:U:9:VAL:HG11  | 30:U:14:PHE:CD1    | 2.54                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 35:Z:36:SER:OG    | 35:Z:38:ASP:OD1   | 2.37                     | 0.43              |
| 52:r:108:ALA:O    | 52:r:112:GLN:HG2  | 2.18                     | 0.43              |
| 65:AE:80:ASP:N    | 65:AE:81:GLU:OE1  | 2.51                     | 0.43              |
| 66:AF:105:LYS:HB2 | 66:AF:105:LYS:HE3 | 1.83                     | 0.43              |
| 2:1:1165:A:H2'    | 2:1:1166:A:C8     | 2.54                     | 0.42              |
| 2:1:1622:U:O2     | 2:1:1813:G:O6     | 2.37                     | 0.42              |
| 2:1:2719:A:H5'    | 47:m:175:HIS:HA   | 2.00                     | 0.42              |
| 8:8:82:LEU:HD22   | 8:8:141:TYR:OH    | 2.18                     | 0.42              |
| 10:A:516:A:C2'    | 10:A:517:C:H5''   | 2.48                     | 0.42              |
| 10:A:873:U:H2'    | 10:A:874:U:C6     | 2.54                     | 0.42              |
| 10:A:1561:G:H5''  | 10:A:1562:G:OP1   | 2.19                     | 0.42              |
| 19:J:141:ARG:HD2  | 19:J:146:GLU:OE2  | 2.19                     | 0.42              |
| 32:W:59:VAL:HG23  | 32:W:64:GLU:HB2   | 2.00                     | 0.42              |
| 42:g:171:GLY:O    | 42:g:172:ILE:HD13 | 2.19                     | 0.42              |
| 42:g:181:GLN:HE21 | 42:g:190:LEU:HB2  | 1.84                     | 0.42              |
| 56:v:114:ARG:CG   | 56:v:137:PRO:HG3  | 2.49                     | 0.42              |
| 2:1:1062:G:H2'    | 2:1:1063:U:H6     | 1.84                     | 0.42              |
| 2:1:1689:C:O2'    | 2:1:1768:U:O2'    | 2.26                     | 0.42              |
| 2:1:3085:A:H2'    | 2:1:3086:A:O4'    | 2.19                     | 0.42              |
| 10:A:127:G:N7     | 17:H:202:ARG:NH2  | 2.67                     | 0.42              |
| 10:A:149:G:H2'    | 10:A:150:U:C6     | 2.54                     | 0.42              |
| 10:A:481:A:H2'    | 10:A:482:C:H4'    | 2.01                     | 0.42              |
| 10:A:1396:A:H5''  | 28:R:117:VAL:HG13 | 2.01                     | 0.42              |
| 13:D:36:LEU:O     | 13:D:40:VAL:HG23  | 2.19                     | 0.42              |
| 16:G:117:ALA:O    | 16:G:118:LEU:C    | 2.62                     | 0.42              |
| 20:K:50:SER:O     | 20:K:54:ARG:HG3   | 2.19                     | 0.42              |
| 20:K:123:HIS:O    | 20:K:127:VAL:HG23 | 2.20                     | 0.42              |
| 26:Q:52:LYS:N     | 26:Q:53:PRO:HD2   | 2.35                     | 0.42              |
| 42:g:181:GLN:NE2  | 42:g:190:LEU:HB2  | 2.33                     | 0.42              |
| 42:g:182:TYR:HE1  | 42:g:187:HIS:HB3  | 1.84                     | 0.42              |
| 44:j:137:ILE:HD11 | 44:j:149:LYS:HB2  | 2.01                     | 0.42              |
| 70:AJ:53:GLU:O    | 70:AJ:57:ILE:HG12 | 2.19                     | 0.42              |
| 2:1:912:G:N1      | 44:j:207:VAL:HG11 | 2.34                     | 0.42              |
| 2:1:1108:A:H2'    | 2:1:1109:G:C8     | 2.53                     | 0.42              |
| 2:1:2408:A:H2'    | 2:1:2409:C:C6     | 2.53                     | 0.42              |
| 2:1:2749:G:C2     | 62:AB:60:TYR:HE1  | 2.36                     | 0.42              |
| 2:1:2848:C:O4'    | 78:AT:77:A:H1'    | 2.19                     | 0.42              |
| 2:1:2972:A:H2'    | 2:1:2973:U:C6     | 2.54                     | 0.42              |
| 10:A:446:C:H2'    | 10:A:447:C:H6     | 1.82                     | 0.42              |
| 16:G:118:LEU:HD13 | 16:G:129:PRO:HB2  | 2.01                     | 0.42              |
| 24:O:55:ARG:HH22  | 38:c:51:GLN:NE2   | 2.18                     | 0.42              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 37:b:51:ARG:O    | 37:b:55:GLU:HG2    | 2.18                     | 0.42              |
| 43:h:62:PHE:HD2  | 43:h:93:TRP:CE3    | 2.37                     | 0.42              |
| 1:0:162:LEU:HD23 | 1:0:162:LEU:HA     | 1.87                     | 0.42              |
| 2:1:254:A:H2'    | 2:1:255:A:O4'      | 2.19                     | 0.42              |
| 2:1:1451:U:H1'   | 65:AE:25:LYS:HE3   | 2.01                     | 0.42              |
| 2:1:1494:A:H2'   | 2:1:1495:U:C6      | 2.54                     | 0.42              |
| 2:1:1690:U:O2'   | 2:1:1691:U:H5'     | 2.19                     | 0.42              |
| 2:1:2077:A:O2'   | 2:1:2078:A:H5'     | 2.20                     | 0.42              |
| 2:1:2965:G:H2'   | 2:1:3114:A:H61     | 1.83                     | 0.42              |
| 2:1:3066:A:H2'   | 2:1:3067:U:C6      | 2.54                     | 0.42              |
| 6:6:104:ASN:OD1  | 6:6:105:PRO:HD2    | 2.19                     | 0.42              |
| 10:A:213:A:H2'   | 10:A:214:U:C6      | 2.54                     | 0.42              |
| 10:A:959:A:H4'   | 24:O:112:LYS:NZ    | 2.34                     | 0.42              |
| 10:A:1370:A:H2'  | 10:A:1371:G:O4'    | 2.20                     | 0.42              |
| 13:D:62:GLN:HA   | 13:D:65:ASP:OD1    | 2.19                     | 0.42              |
| 16:G:208:SER:HB3 | 16:G:211:ILE:HG12  | 2.01                     | 0.42              |
| 18:I:33:GLU:OE1  | 18:I:33:GLU:N      | 2.53                     | 0.42              |
| 18:I:147:LYS:HE3 | 18:I:149:LEU:HD21  | 2.02                     | 0.42              |
| 26:Q:58:LYS:HG2  | 26:Q:61:ARG:NH2    | 2.28                     | 0.42              |
| 58:x:10:ASN:ND2  | 58:x:13:LYS:HG3    | 2.35                     | 0.42              |
| 59:y:175:ALA:O   | 62:AB:51:GLY:HA2   | 2.20                     | 0.42              |
| 2:1:551:U:H2'    | 2:1:552:G:O4'      | 2.19                     | 0.42              |
| 2:1:635:C:C2     | 2:1:636:C:C5       | 3.07                     | 0.42              |
| 2:1:771:A:H62    | 81:1:3407:GET:H531 | 1.84                     | 0.42              |
| 2:1:1287:A:H2'   | 2:1:1288:C:O4'     | 2.19                     | 0.42              |
| 2:1:1344:U:H5'   | 2:1:1347:U:OP1     | 2.19                     | 0.42              |
| 5:4:6:U:H2'      | 5:4:7:U:H6         | 1.85                     | 0.42              |
| 5:4:68:A:H2'     | 5:4:69:U:O4'       | 2.19                     | 0.42              |
| 6:6:23:MET:HE3   | 6:6:100:GLY:HA3    | 2.02                     | 0.42              |
| 10:A:295:U:OP1   | 15:F:37:LYS:HE3    | 2.20                     | 0.42              |
| 10:A:553:A:H2'   | 10:A:554:A:C8      | 2.55                     | 0.42              |
| 13:D:225:TRP:CD2 | 33:X:68:ARG:HD3    | 2.54                     | 0.42              |
| 18:I:110:ARG:HA  | 18:I:113:THR:HG23  | 2.02                     | 0.42              |
| 39:d:14:LYS:HD2  | 39:d:29:ARG:HH12   | 1.83                     | 0.42              |
| 54:t:49:ARG:HD2  | 69:AI:116:PHE:CE2  | 2.54                     | 0.42              |
| 78:PT:11:A:H2'   | 78:PT:12:G:H8      | 1.85                     | 0.42              |
| 78:PT:65:G:H2'   | 78:PT:66:C:H6      | 1.84                     | 0.42              |
| 78:AT:24:C:H2'   | 78:AT:25:U:C6      | 2.55                     | 0.42              |
| 2:1:621:U:H2'    | 2:1:622:G:C8       | 2.55                     | 0.42              |
| 2:1:771:A:N6     | 81:1:3407:GET:H531 | 2.35                     | 0.42              |
| 2:1:844:A:C5     | 2:1:845:C:H1'      | 2.54                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:1:929:A:C2      | 46:l:99:ARG:NH2   | 2.87                     | 0.42              |
| 2:1:1093:G:H4'    | 3:2:129:LYS:HG2   | 2.01                     | 0.42              |
| 2:1:1757:A:O2'    | 2:1:1759:U:OP2    | 2.29                     | 0.42              |
| 2:1:1923:G:C8     | 77:AQ:16:VAL:HG12 | 2.55                     | 0.42              |
| 2:1:2325:U:H2'    | 2:1:2326:A:O4'    | 2.18                     | 0.42              |
| 2:1:2800:G:H5'    | 52:r:8:CYS:SG     | 2.59                     | 0.42              |
| 10:A:1379:C:H2'   | 10:A:1380:G:H8    | 1.84                     | 0.42              |
| 10:A:1388:G:OP1   | 29:S:4:VAL:HA     | 2.19                     | 0.42              |
| 10:A:1526:G:H1    | 27:T:26:ILE:HG23  | 1.84                     | 0.42              |
| 27:T:44:ASN:ND2   | 27:T:48:LYS:HE3   | 2.34                     | 0.42              |
| 29:S:32:LYS:HE3   | 29:S:48:ASN:HD21  | 1.83                     | 0.42              |
| 34:Y:142:LYS:HD2  | 34:Y:143:PRO:HD2  | 2.01                     | 0.42              |
| 45:k:292:ALA:HB2  | 45:k:302:LYS:HD2  | 2.01                     | 0.42              |
| 47:m:97:ALA:O     | 47:m:101:VAL:HG23 | 2.19                     | 0.42              |
| 52:r:150:GLU:O    | 52:r:154:ARG:HG3  | 2.19                     | 0.42              |
| 55:u:109:GLU:O    | 55:u:113:VAL:HG23 | 2.19                     | 0.42              |
| 57:w:62:ALA:HA    | 57:w:71:PRO:HD2   | 2.02                     | 0.42              |
| 64:AD:15:LYS:HZ3  | 64:AD:105:SER:HB2 | 1.84                     | 0.42              |
| 67:AG:38:PRO:O    | 67:AG:42:LYS:HG3  | 2.19                     | 0.42              |
| 1:0:8:GLN:HG2     | 1:0:62:ASN:HB2    | 2.01                     | 0.42              |
| 2:1:621:U:H2'     | 2:1:622:G:H8      | 1.85                     | 0.42              |
| 2:1:1330:U:H2'    | 2:1:1331:U:C6     | 2.55                     | 0.42              |
| 2:1:2072:C:H2'    | 2:1:2073:G:H8     | 1.85                     | 0.42              |
| 2:1:2130:A:H2'    | 2:1:2131:U:C6     | 2.55                     | 0.42              |
| 2:1:2507:A:H2'    | 2:1:2508:G:O4'    | 2.19                     | 0.42              |
| 2:1:2550:C:H2'    | 2:1:2551:G:O4'    | 2.20                     | 0.42              |
| 2:1:2627:U:H4'    | 2:1:2628:A:O4'    | 2.20                     | 0.42              |
| 4:3:107:A:H2'     | 4:3:108:U:C6      | 2.55                     | 0.42              |
| 7:7:18:GLY:HA3    | 7:7:31:PHE:O      | 2.19                     | 0.42              |
| 10:A:938:G:H2'    | 10:A:939:G:C8     | 2.54                     | 0.42              |
| 10:A:1084:U:OP1   | 33:X:71:LYS:NZ    | 2.51                     | 0.42              |
| 10:A:1226:G:H2'   | 10:A:1227:A:C8    | 2.54                     | 0.42              |
| 11:B:18:LEU:HD11  | 29:S:102:ILE:HG21 | 2.01                     | 0.42              |
| 14:E:114:LEU:HD23 | 14:E:115:PRO:O    | 2.20                     | 0.42              |
| 14:E:134:GLY:HA3  | 14:E:157:PHE:O    | 2.20                     | 0.42              |
| 19:J:31:ARG:HD2   | 19:J:56:ARG:HH22  | 1.84                     | 0.42              |
| 24:O:30:SER:O     | 24:O:34:VAL:HG23  | 2.20                     | 0.42              |
| 31:V:56:ARG:HG2   | 31:V:88:ARG:CZ    | 2.50                     | 0.42              |
| 38:c:73:LEU:HD21  | 38:c:79:PHE:HB3   | 2.01                     | 0.42              |
| 46:l:326:LEU:HD23 | 46:l:326:LEU:HA   | 1.85                     | 0.42              |
| 48:n:138:GLN:HE21 | 48:n:142:ASP:CG   | 2.28                     | 0.42              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 54:t:186:GLU:O    | 54:t:190:LYS:HG2 | 2.19                     | 0.42              |
| 2:1:569:U:H2'     | 2:1:570:A:H8     | 1.85                     | 0.42              |
| 2:1:1396:U:H2'    | 2:1:1397:G:O4'   | 2.20                     | 0.42              |
| 2:1:1562:G:H2'    | 2:1:1563:A:O4'   | 2.19                     | 0.42              |
| 2:1:2810:A:H4'    | 52:r:74:LYS:HD2  | 2.00                     | 0.42              |
| 2:1:2853:C:H2'    | 2:1:2854:U:C6    | 2.55                     | 0.42              |
| 2:1:3297:U:H2'    | 2:1:3298:G:O4'   | 2.20                     | 0.42              |
| 2:1:3318:G:H5''   | 2:1:3319:U:H4'   | 2.02                     | 0.42              |
| 5:4:57:C:H4'      | 5:4:63:G:N7      | 2.35                     | 0.42              |
| 8:8:71:THR:O      | 8:8:75:LYS:HG3   | 2.19                     | 0.42              |
| 10:A:58:U:OP1     | 10:A:454:G:O2'   | 2.35                     | 0.42              |
| 10:A:260:U:O2'    | 10:A:261:C:H5'   | 2.20                     | 0.42              |
| 10:A:788:A:C8     | 33:X:107:SER:HA  | 2.55                     | 0.42              |
| 14:E:60:LEU:HA    | 14:E:64:GLY:HA2  | 2.02                     | 0.42              |
| 26:Q:15:PHE:HD2   | 26:Q:22:LEU:HD21 | 1.84                     | 0.42              |
| 42:g:163:CYS:O    | 42:g:165:ALA:N   | 2.52                     | 0.42              |
| 43:h:150:ASP:O    | 43:h:170:SER:OG  | 2.38                     | 0.42              |
| 45:k:46:PHE:CZ    | 45:k:84:MET:HG3  | 2.55                     | 0.42              |
| 50:p:172:LYS:HG2  | 50:p:227:TYR:CD2 | 2.54                     | 0.42              |
| 55:u:120:ARG:HH12 | 57:w:187:ALA:HA  | 1.84                     | 0.42              |
| 67:AG:42:LYS:HA   | 67:AG:45:LEU:HG  | 2.01                     | 0.42              |
| 78:AT:2:G:H2'     | 78:AT:3:C:O4'    | 2.19                     | 0.42              |
| 2:1:441:U:OP1     | 66:AF:3:THR:HG21 | 2.19                     | 0.42              |
| 2:1:696:U:H2'     | 2:1:697:A:O4'    | 2.20                     | 0.42              |
| 2:1:2785:A:H2'    | 2:1:2786:G:O4'   | 2.20                     | 0.42              |
| 10:A:402:G:H2'    | 10:A:403:C:H6    | 1.85                     | 0.42              |
| 10:A:885:A:OP1    | 25:P:38:THR:OG1  | 2.35                     | 0.42              |
| 10:A:943:U:OP2    | 38:c:20:LYS:NZ   | 2.40                     | 0.42              |
| 10:A:1715:U:H2'   | 10:A:1716:C:C6   | 2.54                     | 0.42              |
| 11:B:4:PRO:HB3    | 32:W:41:GLU:OE1  | 2.19                     | 0.42              |
| 11:B:206:ASP:HB2  | 11:B:208:GLU:CD  | 2.45                     | 0.42              |
| 12:C:71:ALA:HB2   | 12:C:80:SER:HA   | 2.02                     | 0.42              |
| 25:P:82:GLY:HA3   | 25:P:115:PRO:HD2 | 2.02                     | 0.42              |
| 28:R:45:PHE:CD1   | 28:R:48:TYR:HD2  | 2.38                     | 0.42              |
| 38:c:34:ASP:O     | 38:c:79:PHE:HA   | 2.20                     | 0.42              |
| 43:h:70:GLN:HG2   | 43:h:112:LEU:CB  | 2.49                     | 0.42              |
| 48:n:39:LEU:HD11  | 48:n:53:TYR:HB2  | 2.02                     | 0.42              |
| 50:p:69:ARG:HD3   | 50:p:238:ILE:O   | 2.20                     | 0.42              |
| 78:PT:21:U:H2'    | 78:PT:22:A:H5'   | 2.02                     | 0.42              |
| 78:AT:28:U:H2'    | 78:AT:29:C:C6    | 2.55                     | 0.42              |
| 2:1:1612:U:H2'    | 2:1:1613:G:C8    | 2.55                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:1:2373:G:H5''   | 45:k:255:TRP:CD1  | 2.55                     | 0.42              |
| 10:A:160:A:H2'    | 10:A:161:G:N3     | 2.35                     | 0.42              |
| 10:A:255:A:N3     | 19:J:64:ASN:ND2   | 2.67                     | 0.42              |
| 10:A:1151:A:H5''  | 16:G:101:GLY:HA2  | 2.02                     | 0.42              |
| 10:A:1502:A:O2'   | 10:A:1504:U:OP2   | 2.23                     | 0.42              |
| 11:B:15:LYS:HZ1   | 29:S:117:ILE:HD11 | 1.84                     | 0.42              |
| 11:B:198:MET:CE   | 11:B:200:ASP:HB2  | 2.48                     | 0.42              |
| 14:E:171:ILE:HG12 | 14:E:188:LYS:HG2  | 2.02                     | 0.42              |
| 18:I:36:PRO:HG2   | 18:I:37:LEU:HD12  | 2.02                     | 0.42              |
| 20:K:62:ARG:CZ    | 20:K:68:LYS:HD3   | 2.49                     | 0.42              |
| 21:L:17:GLN:HA    | 21:L:89:LEU:HD13  | 2.01                     | 0.42              |
| 22:M:71:LEU:HD22  | 22:M:88:ARG:CZ    | 2.49                     | 0.42              |
| 26:Q:73:PRO:HG2   | 26:Q:93:VAL:HG12  | 2.02                     | 0.42              |
| 30:U:49:GLU:HG3   | 30:U:52:THR:HG22  | 2.01                     | 0.42              |
| 43:h:130:LYS:HG2  | 43:h:151:TRP:N    | 2.27                     | 0.42              |
| 61:AA:5:ILE:HG23  | 61:AA:25:ILE:HD13 | 2.01                     | 0.42              |
| 68:AH:58:ARG:HD3  | 68:AH:59:PRO:CD   | 2.45                     | 0.42              |
| 68:AH:58:ARG:CD   | 68:AH:59:PRO:HD2  | 2.43                     | 0.42              |
| 2:1:156:A:N7      | 70:AJ:25:ILE:HG12 | 2.35                     | 0.41              |
| 2:1:358:G:N2      | 2:1:361:A:OP2     | 2.51                     | 0.41              |
| 2:1:1062:G:H2'    | 2:1:1063:U:C6     | 2.55                     | 0.41              |
| 2:1:2354:G:H2'    | 2:1:2355:G:C8     | 2.55                     | 0.41              |
| 2:1:2692:G:OP1    | 59:y:180:ARG:NH1  | 2.50                     | 0.41              |
| 2:1:3241:G:O2'    | 58:x:175:ARG:HD2  | 2.20                     | 0.41              |
| 4:3:4:U:H2'       | 4:3:5:G:H8        | 1.85                     | 0.41              |
| 8:8:67:ILE:HD12   | 8:8:121:LYS:HG3   | 2.00                     | 0.41              |
| 8:8:108:LEU:HD23  | 8:8:125:ARG:HD3   | 2.02                     | 0.41              |
| 10:A:196:A:C2'    | 10:A:197:G:H5'    | 2.50                     | 0.41              |
| 10:A:561:U:H4'    | 41:f:17:GLN:OE1   | 2.20                     | 0.41              |
| 10:A:1403:A:H2'   | 10:A:1404:G:O4'   | 2.20                     | 0.41              |
| 10:A:1555:C:H1'   | 10:A:1556:A:OP2   | 2.20                     | 0.41              |
| 15:F:42:LEU:N     | 15:F:84:ALA:O     | 2.47                     | 0.41              |
| 17:H:7:TYR:CE2    | 17:H:9:ALA:HB3    | 2.55                     | 0.41              |
| 27:T:7:GLU:HG3    | 36:a:42:LEU:O     | 2.20                     | 0.41              |
| 31:V:22:ARG:NH1   | 31:V:91:ASP:OD1   | 2.53                     | 0.41              |
| 34:Y:55:GLU:HG2   | 34:Y:56:LYS:N     | 2.34                     | 0.41              |
| 36:a:65:LEU:HD11  | 36:a:80:LEU:HD21  | 2.02                     | 0.41              |
| 38:c:42:ASN:C     | 38:c:42:ASN:ND2   | 2.73                     | 0.41              |
| 41:f:41:THR:HA    | 41:f:45:VAL:HB    | 2.01                     | 0.41              |
| 44:j:49:ILE:HD11  | 44:j:60:LYS:HE2   | 2.02                     | 0.41              |
| 2:1:559:C:H2'     | 2:1:560:C:H6      | 1.85                     | 0.41              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 2:1:563:U:H2'       | 2:1:564:G:H8        | 1.85                     | 0.41              |
| 2:1:924:C:H41       | 81:1:3412:GET:H713  | 1.85                     | 0.41              |
| 2:1:3021:A:C5       | 45:k:75:ALA:HB2     | 2.54                     | 0.41              |
| 4:3:84:A:H2'        | 4:3:85:G:C8         | 2.55                     | 0.41              |
| 8:8:47:GLN:HG2      | 69:AI:70:TYR:OH     | 2.20                     | 0.41              |
| 10:A:720:C:H1'      | 10:A:721:C:H5       | 1.85                     | 0.41              |
| 10:A:1204:A:H62     | 10:A:1249:G:N2      | 2.15                     | 0.41              |
| 10:A:1241:A:H5'     | 21:L:5:LYS:NZ       | 2.35                     | 0.41              |
| 10:A:1725:U:H2'     | 10:A:1726:C:C6      | 2.55                     | 0.41              |
| 11:B:75:VAL:HG23    | 11:B:86:VAL:HB      | 2.02                     | 0.41              |
| 16:G:144:GLU:HB2    | 16:G:218:GLU:HG3    | 2.02                     | 0.41              |
| 24:O:62:GLN:O       | 24:O:65:VAL:HG22    | 2.20                     | 0.41              |
| 31:V:25:LEU:HB2     | 31:V:113:VAL:HG12   | 2.01                     | 0.41              |
| 31:V:41:ILE:HG23    | 31:V:51:LYS:HE2     | 2.02                     | 0.41              |
| 44:j:27:ALA:HB1     | 44:j:77:ILE:HG13    | 2.02                     | 0.41              |
| 46:l:227:GLU:OE1    | 46:l:238:GLN:HG2    | 2.20                     | 0.41              |
| 1:0:113:ARG:NH1     | 2:1:1207:U:O2'      | 2.52                     | 0.41              |
| 2:1:679:U:C6        | 46:l:116:HIS:HB2    | 2.55                     | 0.41              |
| 2:1:1116:A:H2'      | 2:1:1117:U:C6       | 2.55                     | 0.41              |
| 5:4:38:U:O2'        | 69:AI:83:LYS:HE2    | 2.21                     | 0.41              |
| 10:A:57:G:OP1       | 35:Z:112:LYS:NZ     | 2.35                     | 0.41              |
| 10:A:66:U:H5'       | 17:H:173:PRO:HA     | 2.02                     | 0.41              |
| 10:A:336:C:H2'      | 10:A:337:C:C6       | 2.54                     | 0.41              |
| 10:A:904:A:H2'      | 10:A:905:C:C6       | 2.55                     | 0.41              |
| 10:A:1218:G:H1      | 10:A:1237:C:H5      | 1.68                     | 0.41              |
| 10:A:1382:U:H2'     | 10:A:1383:U:C6      | 2.56                     | 0.41              |
| 10:A:1503:A:O2'     | 10:A:1504:U:H5'     | 2.19                     | 0.41              |
| 10:A:1522:U:O4      | 16:G:187:ILE:HA     | 2.20                     | 0.41              |
| 12:C:38:PHE:CE1     | 12:C:189:ILE:HD11   | 2.54                     | 0.41              |
| 12:C:82:ARG:HD2     | 12:C:103:LEU:HD11   | 2.02                     | 0.41              |
| 20:K:30:LEU:HD21    | 20:K:102:GLU:HG3    | 2.03                     | 0.41              |
| 23:N:42:ALA:HB2     | 23:N:124:LYS:HD3    | 2.02                     | 0.41              |
| 24:O:56:ASP:OD2     | 38:c:52:THR:HG22    | 2.20                     | 0.41              |
| 30:U:50:ALA:HA      | 30:U:53:TRP:HD1     | 1.85                     | 0.41              |
| 34:Y:89:ASN:HB2     | 34:Y:92:CYS:SG      | 2.61                     | 0.41              |
| 43:h:44:LYS:O       | 43:h:59:LYS:N       | 2.42                     | 0.41              |
| 45:k:108:GLU:HG3    | 45:k:137:TYR:CG     | 2.56                     | 0.41              |
| 68:AH:103:ARG:O     | 68:AH:107:GLU:HG3   | 2.20                     | 0.41              |
| 72:AL:30[B]:LYS:HB3 | 72:AL:30[B]:LYS:HE3 | 1.75                     | 0.41              |
| 78:PT:51:U:H2'      | 78:PT:52:C:C6       | 2.55                     | 0.41              |
| 2:1:707:A:H2'       | 2:1:708:A:O4'       | 2.21                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:1:1177:U:O4     | 57:w:19:ARG:HA    | 2.19                     | 0.41              |
| 2:1:2881:U:H2'    | 2:1:2882:A:O4'    | 2.21                     | 0.41              |
| 10:A:1:U:H5''     | 13:D:171:LYS:NZ   | 2.36                     | 0.41              |
| 10:A:148:C:H4'    | 17:H:132:ARG:HH22 | 1.85                     | 0.41              |
| 10:A:750:G:C6     | 20:K:146:PHE:CZ   | 3.08                     | 0.41              |
| 10:A:1037:U:O2'   | 10:A:1038:G:N2    | 2.54                     | 0.41              |
| 10:A:1051:C:H5''  | 12:C:151:LYS:HE3  | 2.02                     | 0.41              |
| 10:A:1475:U:OP1   | 14:E:10:LYS:HE3   | 2.21                     | 0.41              |
| 12:C:52:THR:HG22  | 12:C:55:LYS:HB3   | 2.03                     | 0.41              |
| 16:G:42:LEU:HB2   | 16:G:48:PHE:HE2   | 1.86                     | 0.41              |
| 20:K:169:ALA:HB1  | 20:K:173:LYS:HB3  | 2.02                     | 0.41              |
| 30:U:6:VAL:HB     | 30:U:66:TYR:CE1   | 2.56                     | 0.41              |
| 35:Z:23:PHE:HE1   | 35:Z:75:ILE:HG12  | 1.84                     | 0.41              |
| 44:j:140:ASN:ND2  | 44:j:143:GLU:OE1  | 2.53                     | 0.41              |
| 46:l:113:LYS:CG   | 56:v:202:TYR:HB3  | 2.50                     | 0.41              |
| 47:m:83:LEU:HB3   | 47:m:88:ILE:HB    | 2.01                     | 0.41              |
| 49:o:84:VAL:O     | 49:o:112:GLY:HA2  | 2.20                     | 0.41              |
| 59:y:63:SER:OG    | 59:y:90:ASP:HB2   | 2.20                     | 0.41              |
| 60:z:17:VAL:HG11  | 60:z:52:LYS:HD2   | 2.02                     | 0.41              |
| 60:z:166:ASN:C    | 60:z:166:ASN:HD22 | 2.26                     | 0.41              |
| 62:AB:75:LEU:HD11 | 62:AB:134:ALA:HA  | 2.03                     | 0.41              |
| 71:AK:54:LYS:O    | 71:AK:58:THR:HB   | 2.21                     | 0.41              |
| 2:1:602:A:H2'     | 2:1:603:C:C6      | 2.55                     | 0.41              |
| 2:1:1426:U:H2'    | 62:AB:9:ARG:HH22  | 1.84                     | 0.41              |
| 2:1:2181:U:H2'    | 2:1:2182:C:H6     | 1.85                     | 0.41              |
| 10:A:142:G:O2'    | 10:A:143:A:O5'    | 2.35                     | 0.41              |
| 10:A:508:G:H2'    | 10:A:509:A:O4'    | 2.20                     | 0.41              |
| 10:A:605:G:H5'    | 10:A:611:G:N2     | 2.35                     | 0.41              |
| 10:A:680:C:C2     | 10:A:681:C:C5     | 3.08                     | 0.41              |
| 10:A:918:A:OP2    | 37:b:37:LYS:HE3   | 2.20                     | 0.41              |
| 10:A:1293:G:H2'   | 10:A:1294:C:C6    | 2.55                     | 0.41              |
| 14:E:219:ILE:HG23 | 14:E:222:PRO:HG3  | 2.03                     | 0.41              |
| 20:K:92:LYS:O     | 20:K:93:LEU:HB2   | 2.20                     | 0.41              |
| 25:P:94:GLN:CD    | 37:b:46:GLU:H     | 2.28                     | 0.41              |
| 28:R:46:LYS:HE2   | 28:R:78:TYR:CZ    | 2.54                     | 0.41              |
| 28:R:59:PHE:CZ    | 28:R:88:LEU:HD13  | 2.56                     | 0.41              |
| 29:S:84:TYR:CE1   | 29:S:86:PRO:HG3   | 2.54                     | 0.41              |
| 31:V:101:ARG:HA   | 31:V:104:GLN:HG3  | 2.01                     | 0.41              |
| 33:X:20:THR:O     | 33:X:20:THR:HG22  | 2.20                     | 0.41              |
| 42:g:168:CYS:SG   | 42:g:169:GLY:N    | 2.94                     | 0.41              |
| 43:h:124:VAL:HG22 | 43:h:157:ILE:HD11 | 2.03                     | 0.41              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 45:k:90:VAL:HG22   | 45:k:104:THR:HG23 | 2.01                     | 0.41              |
| 46:l:36:VAL:HG21   | 46:l:245:LEU:HD21 | 2.03                     | 0.41              |
| 65:AE:26:LYS:HA    | 65:AE:29:PRO:HG2  | 2.01                     | 0.41              |
| 1:0:95:ARG:HG2     | 1:0:95:ARG:NH1    | 2.35                     | 0.41              |
| 2:1:1077:U:H5'     | 2:1:1078:U:C5     | 2.55                     | 0.41              |
| 2:1:2391:A:H2'     | 2:1:2392:G:H8     | 1.86                     | 0.41              |
| 10:A:197:G:H2'     | 10:A:198:G:O4'    | 2.21                     | 0.41              |
| 10:A:411:U:H2'     | 10:A:412:C:H6     | 1.86                     | 0.41              |
| 10:A:483:A:H2'     | 10:A:484:G:C8     | 2.54                     | 0.41              |
| 10:A:507:G:H2'     | 10:A:508:G:C8     | 2.55                     | 0.41              |
| 10:A:734:U:H2'     | 10:A:735:U:H6     | 1.86                     | 0.41              |
| 10:A:740:A:O2'     | 10:A:741:A:OP1    | 2.36                     | 0.41              |
| 10:A:1211:A:O2'    | 10:A:1241:A:N1    | 2.39                     | 0.41              |
| 10:A:1381:A:H2'    | 10:A:1382:U:C6    | 2.55                     | 0.41              |
| 10:A:1435:U:H2'    | 10:A:1436:U:C6    | 2.55                     | 0.41              |
| 11:B:58:VAL:O      | 11:B:62:ARG:HG3   | 2.21                     | 0.41              |
| 15:F:107:GLY:CA    | 15:F:189:LEU:HD23 | 2.50                     | 0.41              |
| 18:I:162:LEU:O     | 18:I:166:GLN:HG3  | 2.21                     | 0.41              |
| 19:J:166:PHE:CZ    | 19:J:171:LEU:HD11 | 2.56                     | 0.41              |
| 20:K:30:LEU:HA     | 20:K:30:LEU:HD23  | 1.84                     | 0.41              |
| 20:K:38:ASN:OD1    | 20:K:41:GLU:HG3   | 2.21                     | 0.41              |
| 21:L:50:THR:HG21   | 21:L:57:THR:OG1   | 2.20                     | 0.41              |
| 28:R:41:GLU:OE1    | 28:R:41:GLU:N     | 2.54                     | 0.41              |
| 29:S:107:ALA:O     | 29:S:111:LYS:HG2  | 2.21                     | 0.41              |
| 32:W:37:ALA:HA     | 32:W:50:ASN:OD1   | 2.21                     | 0.41              |
| 43:h:26:THR:HG23   | 43:h:29:HIS:H     | 1.85                     | 0.41              |
| 43:h:84:ALA:HB1    | 43:h:111:VAL:HG23 | 2.02                     | 0.41              |
| 54:t:56:PRO:HG3    | 54:t:74:GLY:C     | 2.46                     | 0.41              |
| 76:AP:104:LEU:HD22 | 76:AP:106:PHE:HD1 | 1.86                     | 0.41              |
| 2:1:516:U:OP1      | 46:l:352:PRO:HD2  | 2.19                     | 0.41              |
| 2:1:1313:A:O2'     | 2:1:1314:A:H3'    | 2.20                     | 0.41              |
| 2:1:1593:C:H5'     | 2:1:1692:A:H1'    | 2.02                     | 0.41              |
| 2:1:2208:C:H2'     | 2:1:2209:C:O4'    | 2.21                     | 0.41              |
| 2:1:2245:C:H2'     | 2:1:2246:U:O4'    | 2.20                     | 0.41              |
| 2:1:2719:A:H2'     | 2:1:2720:A:C8     | 2.55                     | 0.41              |
| 10:A:477:C:H2'     | 10:A:478:G:H8     | 1.85                     | 0.41              |
| 10:A:736:G:H2'     | 10:A:737:A:H8     | 1.84                     | 0.41              |
| 10:A:849:U:H3'     | 33:X:28:ARG:HH22  | 1.86                     | 0.41              |
| 10:A:1176:U:H2'    | 10:A:1177:C:C6    | 2.55                     | 0.41              |
| 10:A:1369:G:H1'    | 10:A:1370:A:O5'   | 2.20                     | 0.41              |
| 11:B:167:LYS:CE    | 11:B:203:PHE:HB3  | 2.50                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 21:L:76:LEU:HD21  | 21:L:80:LEU:HD12   | 2.02                     | 0.41              |
| 25:P:123:ARG:NH1  | 37:b:23:CYS:O      | 2.54                     | 0.41              |
| 39:d:11:LYS:NZ    | 39:d:51:ASN:OD1    | 2.48                     | 0.41              |
| 42:g:183:CYS:HB3  | 42:g:186:CYS:SG    | 2.60                     | 0.41              |
| 56:v:180:PHE:O    | 56:v:184:LYS:HB2   | 2.21                     | 0.41              |
| 62:AB:75:LEU:HD22 | 62:AB:118:LEU:HD11 | 2.03                     | 0.41              |
| 72:AL:40:GLN:HE21 | 72:AL:55:VAL:CG1   | 2.30                     | 0.41              |
| 76:AP:46:LYS:HE3  | 76:AP:54:THR:HB    | 2.03                     | 0.41              |
| 78:PT:36:A:N1     | 79:MR:6:A:N1       | 2.69                     | 0.41              |
| 2:1:106:A:H1'     | 2:1:325:A:N3       | 2.36                     | 0.41              |
| 2:1:299:G:C8      | 70:AJ:30:GLY:HA3   | 2.56                     | 0.41              |
| 2:1:1691:U:O2     | 68:AH:26:PRO:HB3   | 2.21                     | 0.41              |
| 2:1:2232:U:H2'    | 2:1:2239:G:N2      | 2.36                     | 0.41              |
| 2:1:2296:U:H2'    | 2:1:2297:U:O4'     | 2.21                     | 0.41              |
| 10:A:734:U:H2'    | 10:A:735:U:C6      | 2.55                     | 0.41              |
| 10:A:1459:U:O4    | 16:G:180:ARG:HG3   | 2.21                     | 0.41              |
| 10:A:1600:U:C4    | 10:A:1601:A:N1     | 2.89                     | 0.41              |
| 14:E:102:GLN:HB3  | 14:E:123:VAL:HG13  | 2.01                     | 0.41              |
| 16:G:25:LEU:HD23  | 16:G:25:LEU:HA     | 1.90                     | 0.41              |
| 23:N:27:ALA:O     | 23:N:30:VAL:HG13   | 2.21                     | 0.41              |
| 27:T:25:ARG:HE    | 36:a:40:VAL:HB     | 1.86                     | 0.41              |
| 43:h:291:TRP:CZ3  | 43:h:298:LEU:HD13  | 2.56                     | 0.41              |
| 2:1:356:C:O2'     | 46:l:82:GLY:O      | 2.28                     | 0.41              |
| 2:1:982:U:H5'     | 49:o:127:LEU:HD11  | 2.02                     | 0.41              |
| 2:1:989:G:N3      | 2:1:2609:A:H2'     | 2.35                     | 0.41              |
| 2:1:1035:U:H2'    | 2:1:1036:A:C8      | 2.56                     | 0.41              |
| 2:1:1469:G:C4'    | 60:z:26:PRO:HG3    | 2.50                     | 0.41              |
| 2:1:2523:C:H2'    | 2:1:2524:C:C6      | 2.56                     | 0.41              |
| 2:1:2854:U:H2'    | 2:1:2855:U:C6      | 2.56                     | 0.41              |
| 2:1:2866:C:H2'    | 2:1:2867:G:H8      | 1.86                     | 0.41              |
| 2:1:3233:A:OP1    | 48:n:45:ARG:NH2    | 2.48                     | 0.41              |
| 2:1:3233:A:H5''   | 48:n:45:ARG:NH1    | 2.36                     | 0.41              |
| 2:1:3245:A:O2'    | 2:1:3246:C:O5'     | 2.35                     | 0.41              |
| 4:3:26:C:H5''     | 47:m:56:THR:HG21   | 2.02                     | 0.41              |
| 6:6:61:THR:HG22   | 6:6:72:LYS:O       | 2.20                     | 0.41              |
| 10:A:255:A:H1'    | 19:J:73:SER:OG     | 2.21                     | 0.41              |
| 10:A:566:G:OP2    | 34:Y:70:LYS:NZ     | 2.38                     | 0.41              |
| 10:A:750:G:C6     | 20:K:149:ARG:NE    | 2.88                     | 0.41              |
| 10:A:812:C:H2'    | 10:A:813:U:C6      | 2.56                     | 0.41              |
| 10:A:1238:U:H4'   | 42:g:185:LYS:HB2   | 2.03                     | 0.41              |
| 10:A:1396:A:H2'   | 10:A:1397:A:O4'    | 2.19                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:B:201:LEU:HG   | 11:B:202:TYR:H    | 1.86                     | 0.41              |
| 12:C:71:ALA:O     | 12:C:75:GLY:N     | 2.54                     | 0.41              |
| 15:F:247:LEU:HB2  | 15:F:252:GLU:HG2  | 2.03                     | 0.41              |
| 18:I:63:LEU:HD22  | 18:I:90:ALA:HB2   | 2.01                     | 0.41              |
| 18:I:131:ILE:HG23 | 18:I:148:VAL:HG13 | 2.03                     | 0.41              |
| 19:J:39:GLY:O     | 19:J:61:GLU:HG2   | 2.21                     | 0.41              |
| 21:L:17:GLN:O     | 21:L:18:GLU:HG3   | 2.20                     | 0.41              |
| 25:P:7:GLN:OE1    | 25:P:106:ARG:HG3  | 2.21                     | 0.41              |
| 25:P:79:ARG:HH21  | 25:P:115:PRO:HG2  | 1.85                     | 0.41              |
| 30:U:27:LYS:HG3   | 30:U:111:ILE:HD12 | 2.03                     | 0.41              |
| 30:U:65:ILE:HG13  | 30:U:71:VAL:CG2   | 2.50                     | 0.41              |
| 31:V:54:PRO:HA    | 31:V:90:ILE:HG13  | 2.02                     | 0.41              |
| 39:d:11:LYS:NZ    | 39:d:13:ILE:HG22  | 2.36                     | 0.41              |
| 43:h:87:ASP:OD1   | 43:h:89:THR:HG22  | 2.21                     | 0.41              |
| 43:h:175:VAL:O    | 43:h:175:VAL:HG12 | 2.20                     | 0.41              |
| 47:m:235:ASP:HA   | 47:m:238:GLU:OE2  | 2.21                     | 0.41              |
| 48:n:73:VAL:HA    | 48:n:74:PRO:HD3   | 1.93                     | 0.41              |
| 49:o:158:ARG:HG3  | 49:o:201:TRP:CG   | 2.56                     | 0.41              |
| 56:v:48:ALA:O     | 56:v:53:TYR:HB3   | 2.21                     | 0.41              |
| 61:AA:23:VAL:HG12 | 61:AA:45:GLY:HA3  | 2.03                     | 0.41              |
| 2:1:106:A:H2'     | 2:1:107:A:O4'     | 2.21                     | 0.41              |
| 2:1:745:C:H5''    | 63:AC:32:LEU:HD12 | 2.03                     | 0.41              |
| 10:A:815:U:C2     | 10:A:816:U:C6     | 3.09                     | 0.41              |
| 10:A:985:C:H5     | 10:A:988:A:OP2    | 2.03                     | 0.41              |
| 10:A:1110:A:O2'   | 10:A:1763:A:OP1   | 2.33                     | 0.41              |
| 10:A:1581:G:H5'   | 40:e:33:LYS:HD2   | 2.03                     | 0.41              |
| 12:C:168:MET:HA   | 12:C:197:ILE:HD12 | 2.01                     | 0.41              |
| 14:E:124:LEU:O    | 14:E:128:MET:HG2  | 2.21                     | 0.41              |
| 19:J:107:THR:HB   | 19:J:108:PRO:HD3  | 2.02                     | 0.41              |
| 25:P:6:SER:OG     | 25:P:7:GLN:N      | 2.54                     | 0.41              |
| 25:P:56:MET:HB2   | 25:P:95:SER:OG    | 2.21                     | 0.41              |
| 32:W:83:TRP:NE1   | 32:W:87:ARG:HH22  | 2.18                     | 0.41              |
| 33:X:90:THR:O     | 33:X:94:LEU:HB2   | 2.21                     | 0.41              |
| 35:Z:20:ARG:HB3   | 35:Z:76:TYR:CD1   | 2.56                     | 0.41              |
| 35:Z:87:PRO:HG2   | 35:Z:90:ARG:HD3   | 2.03                     | 0.41              |
| 35:Z:90:ARG:HA    | 35:Z:93:ARG:HD2   | 2.03                     | 0.41              |
| 42:g:174:MET:HG2  | 42:g:182:TYR:O    | 2.21                     | 0.41              |
| 43:h:289:LEU:O    | 43:h:289:LEU:HD23 | 2.20                     | 0.41              |
| 48:n:39:LEU:HB3   | 48:n:83:VAL:HG13  | 2.03                     | 0.41              |
| 50:p:244:ASN:HA   | 50:p:247:ILE:HD12 | 2.02                     | 0.41              |
| 1:0:159:SER:HB2   | 2:1:3172:U:O4     | 2.22                     | 0.40              |

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| Atom-1            | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 2:1:564:G:H2'     | 2:1:565:A:H8        | 1.82                     | 0.40              |
| 2:1:1358:C:H2'    | 2:1:1359:A:C8       | 2.56                     | 0.40              |
| 2:1:2413:G:H4'    | 56:v:24:ARG:HH22    | 1.86                     | 0.40              |
| 2:1:2728:C:O4'    | 3:2:49:GLN:HG2      | 2.21                     | 0.40              |
| 2:1:2854:U:H2'    | 2:1:2855:U:O4'      | 2.21                     | 0.40              |
| 2:1:3166:A:H2'    | 2:1:3167:G:H8       | 1.82                     | 0.40              |
| 5:4:146:U:H2'     | 5:4:147:U:C6        | 2.57                     | 0.40              |
| 10:A:484:G:N2     | 10:A:501:G:O6       | 2.42                     | 0.40              |
| 10:A:872:A:H5''   | 25:P:115:PRO:HB3    | 2.02                     | 0.40              |
| 10:A:1158:C:OP1   | 27:T:132:LYS:NZ     | 2.50                     | 0.40              |
| 10:A:1329:A:H2'   | 10:A:1330:A:C8      | 2.56                     | 0.40              |
| 10:A:1345:A:H2'   | 10:A:1346:U:O4'     | 2.21                     | 0.40              |
| 10:A:1656:U:H2'   | 10:A:1657:G:O4'     | 2.21                     | 0.40              |
| 11:B:3:LEU:HD12   | 11:B:4:PRO:HD2      | 2.02                     | 0.40              |
| 18:I:139:LEU:HD11 | 18:I:145:ILE:HD12   | 2.03                     | 0.40              |
| 20:K:28:LEU:HB3   | 41:f:44:PHE:HE2     | 1.85                     | 0.40              |
| 25:P:40:GLY:HA2   | 25:P:49:GLU:HG2     | 2.03                     | 0.40              |
| 26:Q:15:PHE:CZ    | 26:Q:110:GLU:HG3    | 2.56                     | 0.40              |
| 28:R:21:VAL:HG22  | 28:R:64:ILE:HG22    | 2.03                     | 0.40              |
| 29:S:13:SER:OG    | 29:S:57:LEU:HD12    | 2.21                     | 0.40              |
| 30:U:105:VAL:HA   | 30:U:108:LEU:HD12   | 2.03                     | 0.40              |
| 38:c:42:ASN:OD1   | 38:c:56:CYS:SG      | 2.73                     | 0.40              |
| 39:d:64:ARG:O     | 39:d:65:ARG:HD2     | 2.21                     | 0.40              |
| 43:h:43:ILE:HB    | 43:h:45:TRP:HE1     | 1.86                     | 0.40              |
| 50:p:119:GLU:CD   | 50:p:120:GLY:H      | 2.27                     | 0.40              |
| 50:p:163:LEU:HA   | 56:v:7:LEU:HD11     | 2.03                     | 0.40              |
| 55:u:120:ARG:NH1  | 57:w:186:THR:HG23   | 2.35                     | 0.40              |
| 64:AD:24:LYS:HB2  | 64:AD:96:ASP:HB3    | 2.04                     | 0.40              |
| 2:1:277:G:H2'     | 2:1:278:U:C6        | 2.56                     | 0.40              |
| 2:1:757:A:C2      | 2:1:767:A:H1'       | 2.56                     | 0.40              |
| 2:1:943:G:H2'     | 2:1:944:C:C6        | 2.56                     | 0.40              |
| 2:1:1152:C:OP2    | 49:o:92:LYS:NZ      | 2.53                     | 0.40              |
| 2:1:1352:C:H5''   | 2:1:1353:G:C8       | 2.56                     | 0.40              |
| 2:1:1840:C:O2     | 71:AK:9:GLY:HA2     | 2.22                     | 0.40              |
| 2:1:2185:A:C8     | 2:1:2186:A:H2       | 2.39                     | 0.40              |
| 2:1:2342:G:H22    | 2:1:2374:G:H1'      | 1.85                     | 0.40              |
| 2:1:2517:C:H4'    | 2:1:2518:A:H5'      | 2.04                     | 0.40              |
| 5:4:52:A:OP1      | 73:AM:21[B]:ARG:NH1 | 2.39                     | 0.40              |
| 6:6:59:MET:HE3    | 6:6:73:VAL:HG12     | 2.03                     | 0.40              |
| 6:6:80:ARG:HD2    | 6:6:97:ASP:OD1      | 2.22                     | 0.40              |
| 10:A:266:C:O2'    | 10:A:267:G:H5'      | 2.21                     | 0.40              |

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| Atom-1              | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|-------------------|--------------------------|-------------------|
| 10:A:328:G:O2'      | 19:J:33:PRO:HB3   | 2.21                     | 0.40              |
| 10:A:873:U:H2'      | 10:A:874:U:H6     | 1.86                     | 0.40              |
| 10:A:1105:U:H2'     | 10:A:1106:C:C6    | 2.56                     | 0.40              |
| 10:A:1374:A:N6      | 10:A:1397:A:N7    | 2.69                     | 0.40              |
| 10:A:1437:C:P       | 40:e:12:ARG:HH22  | 2.43                     | 0.40              |
| 12:C:101:HIS:ND1    | 12:C:217:LEU:HD23 | 2.37                     | 0.40              |
| 18:I:41:SER:O       | 18:I:57:PHE:HB2   | 2.20                     | 0.40              |
| 23:N:74:LEU:HD11    | 42:g:148:TYR:HB2  | 2.03                     | 0.40              |
| 44:j:112:ILE:HG13   | 77:AQ:79:VAL:HG22 | 2.03                     | 0.40              |
| 47:m:197:LYS:HG3    | 47:m:202:GLY:HA3  | 2.02                     | 0.40              |
| 49:o:143[B]:ARG:HG3 | 49:o:183:ILE:HG21 | 2.04                     | 0.40              |
| 51:q:79:ILE:O       | 51:q:82:VAL:HG12  | 2.21                     | 0.40              |
| 1:0:138[B]:GLN:HA   | 1:0:141:LYS:HB3   | 2.02                     | 0.40              |
| 2:1:88:G:H21        | 2:1:281:G:C4'     | 2.34                     | 0.40              |
| 2:1:394:G:N1        | 2:1:397:A:OP2     | 2.54                     | 0.40              |
| 2:1:1177:U:O4       | 57:w:22:SER:OG    | 2.36                     | 0.40              |
| 2:1:2855:U:H2'      | 2:1:2856:C:H6     | 1.85                     | 0.40              |
| 81:1:3404:GET:H712  | 81:1:3404:GET:N32 | 2.36                     | 0.40              |
| 7:7:35:LYS:HE3      | 7:7:51:TRP:CH2    | 2.57                     | 0.40              |
| 10:A:74:U:O2'       | 10:A:76:A:OP2     | 2.28                     | 0.40              |
| 10:A:216:A:H61      | 10:A:829:A:H1'    | 1.87                     | 0.40              |
| 10:A:331:A:N7       | 19:J:49:ARG:HD3   | 2.36                     | 0.40              |
| 10:A:879:U:H2'      | 25:P:31:LYS:HD2   | 2.03                     | 0.40              |
| 10:A:1330:A:H3'     | 10:A:1333:A:H62   | 1.86                     | 0.40              |
| 10:A:1438:U:C2      | 10:A:1439:G:C8    | 3.10                     | 0.40              |
| 10:A:1444:G:OP2     | 27:T:139:LYS:HB2  | 2.21                     | 0.40              |
| 12:C:29:TRP:HA      | 12:C:46:THR:O     | 2.21                     | 0.40              |
| 12:C:30:PHE:CG      | 12:C:61:LEU:HD21  | 2.57                     | 0.40              |
| 14:E:49:VAL:O       | 14:E:88:TYR:N     | 2.46                     | 0.40              |
| 15:F:180:LEU:HD12   | 15:F:193:GLY:O    | 2.21                     | 0.40              |
| 16:G:108:LEU:HA     | 16:G:111:VAL:HG12 | 2.03                     | 0.40              |
| 17:H:1:MET:HE2      | 17:H:1:MET:HB3    | 1.87                     | 0.40              |
| 17:H:160:ARG:HH21   | 17:H:171:LYS:HD3  | 1.86                     | 0.40              |
| 20:K:123:HIS:CE1    | 41:f:37:ARG:HB2   | 2.56                     | 0.40              |
| 20:K:170:GLY:O      | 20:K:174:ARG:HG3  | 2.21                     | 0.40              |
| 24:O:27:LYS:O       | 24:O:27:LYS:HG3   | 2.21                     | 0.40              |
| 27:T:112:ASP:O      | 27:T:115:ARG:HG2  | 2.21                     | 0.40              |
| 29:S:6:THR:O        | 29:S:10:LYS:HG3   | 2.21                     | 0.40              |
| 31:V:38:ALA:O       | 31:V:42:ARG:HG2   | 2.20                     | 0.40              |
| 36:a:54:VAL:HG23    | 36:a:88:ILE:HG21  | 2.02                     | 0.40              |
| 41:f:4:VAL:HG21     | 78:AT:37:U:O2'    | 2.21                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 42:g:182:TYR:OH   | 42:g:187:HIS:HB3  | 2.21                     | 0.40              |
| 45:k:262:TRP:CD1  | 45:k:262:TRP:H    | 2.39                     | 0.40              |
| 53:s:9:MET:HE3    | 53:s:9:MET:HB3    | 1.98                     | 0.40              |
| 59:y:44:PHE:CD2   | 59:y:134:GLY:HA3  | 2.56                     | 0.40              |
| 66:AF:80:VAL:HG13 | 66:AF:112:LYS:CD  | 2.49                     | 0.40              |
| 67:AG:103:TYR:HA  | 67:AG:104:PRO:C   | 2.46                     | 0.40              |
| 78:PT:20:G:N2     | 78:PT:58:A:H1'    | 2.36                     | 0.40              |
| 78:AT:75:C:H2'    | 78:AT:76:C:O4'    | 2.21                     | 0.40              |
| 2:1:206:U:H2'     | 2:1:207:C:H6      | 1.85                     | 0.40              |
| 2:1:1060:A:H4'    | 2:1:1061:A:O5'    | 2.21                     | 0.40              |
| 2:1:1286:A:H2'    | 2:1:1287:A:H8     | 1.87                     | 0.40              |
| 2:1:1491:U:C5     | 2:1:1831:A:N1     | 2.83                     | 0.40              |
| 2:1:2883:A:H4'    | 2:1:2884:G:C8     | 2.57                     | 0.40              |
| 2:1:2919:G:N3     | 45:k:250:ALA:HB1  | 2.37                     | 0.40              |
| 5:4:111:A:N6      | 71:AK:29:VAL:HG11 | 2.36                     | 0.40              |
| 10:A:72:A:N7      | 17:H:164:LYS:NZ   | 2.68                     | 0.40              |
| 10:A:540:A:OP1    | 41:f:28:LYS:NZ    | 2.42                     | 0.40              |
| 10:A:1032:G:H1    | 10:A:1056:U:H3    | 1.68                     | 0.40              |
| 10:A:1132:A:H2'   | 10:A:1133:C:H6    | 1.86                     | 0.40              |
| 10:A:1276:G:H1    | 10:A:1309:G:N2    | 1.99                     | 0.40              |
| 10:A:1421:G:N7    | 21:L:25:LYS:NZ    | 2.64                     | 0.40              |
| 12:C:70:LEU:HD13  | 12:C:84:ILE:HG13  | 2.02                     | 0.40              |
| 14:E:177:LEU:HD23 | 14:E:182:VAL:HG22 | 2.03                     | 0.40              |
| 16:G:58:LEU:HD22  | 16:G:138:VAL:HA   | 2.04                     | 0.40              |
| 16:G:96:SER:OG    | 16:G:176:THR:HG21 | 2.21                     | 0.40              |
| 21:L:3:ILE:HG22   | 21:L:8:ARG:HB2    | 2.04                     | 0.40              |
| 26:Q:85:VAL:HA    | 26:Q:89:MET:SD    | 2.61                     | 0.40              |
| 28:R:18:VAL:O     | 28:R:66:VAL:HA    | 2.22                     | 0.40              |
| 29:S:18:GLU:HA    | 29:S:71:PHE:HB3   | 2.02                     | 0.40              |
| 30:U:14:PHE:CD2   | 30:U:63:ARG:HD2   | 2.57                     | 0.40              |
| 34:Y:125:VAL:HG12 | 34:Y:126:LYS:HG3  | 2.03                     | 0.40              |
| 35:Z:106:GLN:O    | 35:Z:110:GLN:HG3  | 2.21                     | 0.40              |
| 45:k:58:ARG:O     | 45:k:71:GLU:HA    | 2.21                     | 0.40              |
| 48:n:6:PRO:HB3    | 66:AF:93:TYR:CE1  | 2.56                     | 0.40              |
| 66:AF:33:TRP:CH2  | 66:AF:53:GLN:HG2  | 2.56                     | 0.40              |
| 78:AT:22:A:H61    | 78:AT:47:G:H2'    | 1.86                     | 0.40              |
| 2:1:87:A:H2'      | 2:1:88:G:O4'      | 2.21                     | 0.40              |
| 2:1:922:A:H2'     | 2:1:923:C:H6      | 1.87                     | 0.40              |
| 2:1:3093:U:H1'    | 2:1:3094:A:H5''   | 2.02                     | 0.40              |
| 4:3:31:U:O2'      | 4:3:32:U:H5'      | 2.21                     | 0.40              |
| 5:4:142:C:H2'     | 5:4:143:U:C6      | 2.57                     | 0.40              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 9:9:103:LYS:HA   | 9:9:103:LYS:HD3   | 1.92                     | 0.40              |
| 10:A:126:A:H62   | 10:A:289:G:N2     | 2.14                     | 0.40              |
| 10:A:267:G:N7    | 17:H:186:ARG:NH2  | 2.67                     | 0.40              |
| 10:A:505:U:O2'   | 10:A:506:U:O5'    | 2.37                     | 0.40              |
| 10:A:1155:G:H2'  | 10:A:1155:G:N3    | 2.36                     | 0.40              |
| 10:A:1529:G:N2   | 10:A:1555:C:H1'   | 2.34                     | 0.40              |
| 14:E:98:SER:O    | 14:E:102:GLN:HG2  | 2.21                     | 0.40              |
| 15:F:15:PRO:HG2  | 15:F:18:TRP:CZ2   | 2.57                     | 0.40              |
| 17:H:214:LYS:O   | 17:H:217:HIS:ND1  | 2.54                     | 0.40              |
| 18:I:10:PRO:HB2  | 18:I:14:GLU:HB2   | 2.04                     | 0.40              |
| 20:K:111:THR:O   | 20:K:115:LYS:HG2  | 2.21                     | 0.40              |
| 28:R:47:VAL:HA   | 28:R:81:ARG:HB3   | 2.04                     | 0.40              |
| 50:p:78:GLN:OE1  | 50:p:168:PRO:HG2  | 2.21                     | 0.40              |
| 63:AC:20:GLY:HA3 | 63:AC:21:ILE:HA   | 1.81                     | 0.40              |
| 64:AD:55:LYS:O   | 64:AD:59:GLU:HG2  | 2.22                     | 0.40              |
| 66:AF:44:ARG:HG2 | 66:AF:44:ARG:HH11 | 1.86                     | 0.40              |
| 78:PT:25:U:H2'   | 78:PT:26:C:O4'    | 2.22                     | 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     | 171/172 (99%) | 169 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 3   | 2     | 159/160 (99%) | 157 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 6   | 6     | 129/137 (94%) | 127 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 7   | 7     | 60/155 (39%)  | 60 (100%) | 0       | 0        | 100         | 100 |
| 8   | 8     | 117/142 (82%) | 114 (97%) | 3 (3%)  | 0        | 100         | 100 |
| 9   | 9     | 123/127 (97%) | 119 (97%) | 4 (3%)  | 0        | 100         | 100 |
| 11  | B     | 206/261 (79%) | 191 (93%) | 14 (7%) | 1 (0%)   | 24          | 27  |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 12  | C     | 212/256 (83%) | 197 (93%) | 15 (7%)  | 0        | 100         | 100 |
| 13  | D     | 214/249 (86%) | 204 (95%) | 10 (5%)  | 0        | 100         | 100 |
| 14  | E     | 220/251 (88%) | 204 (93%) | 16 (7%)  | 0        | 100         | 100 |
| 15  | F     | 258/262 (98%) | 248 (96%) | 10 (4%)  | 0        | 100         | 100 |
| 16  | G     | 195/225 (87%) | 178 (91%) | 17 (9%)  | 0        | 100         | 100 |
| 17  | H     | 224/236 (95%) | 217 (97%) | 7 (3%)   | 0        | 100         | 100 |
| 18  | I     | 180/186 (97%) | 166 (92%) | 14 (8%)  | 0        | 100         | 100 |
| 19  | J     | 201/206 (98%) | 196 (98%) | 5 (2%)   | 0        | 100         | 100 |
| 20  | K     | 176/189 (93%) | 164 (93%) | 12 (7%)  | 0        | 100         | 100 |
| 21  | L     | 91/118 (77%)  | 81 (89%)  | 10 (11%) | 0        | 100         | 100 |
| 22  | M     | 139/155 (90%) | 134 (96%) | 5 (4%)   | 0        | 100         | 100 |
| 23  | N     | 65/143 (46%)  | 46 (71%)  | 18 (28%) | 1 (2%)   | 8           | 7   |
| 24  | O     | 148/151 (98%) | 146 (99%) | 2 (1%)   | 0        | 100         | 100 |
| 25  | P     | 124/132 (94%) | 116 (94%) | 8 (6%)   | 0        | 100         | 100 |
| 26  | Q     | 113/142 (80%) | 104 (92%) | 9 (8%)   | 0        | 100         | 100 |
| 27  | T     | 140/145 (97%) | 117 (84%) | 21 (15%) | 2 (1%)   | 9           | 7   |
| 28  | R     | 139/142 (98%) | 126 (91%) | 13 (9%)  | 0        | 100         | 100 |
| 29  | S     | 116/137 (85%) | 104 (90%) | 12 (10%) | 0        | 100         | 100 |
| 30  | U     | 139/145 (96%) | 133 (96%) | 6 (4%)   | 0        | 100         | 100 |
| 31  | V     | 98/119 (82%)  | 95 (97%)  | 3 (3%)   | 0        | 100         | 100 |
| 32  | W     | 85/87 (98%)   | 79 (93%)  | 6 (7%)   | 0        | 100         | 100 |
| 33  | X     | 127/130 (98%) | 122 (96%) | 5 (4%)   | 0        | 100         | 100 |
| 34  | Y     | 141/145 (97%) | 138 (98%) | 3 (2%)   | 0        | 100         | 100 |
| 35  | Z     | 130/135 (96%) | 124 (95%) | 6 (5%)   | 0        | 100         | 100 |
| 36  | a     | 70/105 (67%)  | 64 (91%)  | 6 (9%)   | 0        | 100         | 100 |
| 37  | b     | 96/119 (81%)  | 92 (96%)  | 4 (4%)   | 0        | 100         | 100 |
| 38  | c     | 79/82 (96%)   | 73 (92%)  | 6 (8%)   | 0        | 100         | 100 |
| 39  | d     | 60/67 (90%)   | 51 (85%)  | 9 (15%)  | 0        | 100         | 100 |
| 40  | e     | 53/56 (95%)   | 50 (94%)  | 3 (6%)   | 0        | 100         | 100 |
| 41  | f     | 56/63 (89%)   | 53 (95%)  | 3 (5%)   | 0        | 100         | 100 |
| 42  | g     | 66/193 (34%)  | 48 (73%)  | 17 (26%) | 1 (2%)   | 8           | 7   |

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| Mol | Chain | Analysed       | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|----------------|-----------|----------|----------|-------------|-----|
| 43  | h     | 229/317 (72%)  | 204 (89%) | 25 (11%) | 0        | 100         | 100 |
| 44  | j     | 248/254 (98%)  | 238 (96%) | 10 (4%)  | 0        | 100         | 100 |
| 45  | k     | 385/389 (99%)  | 374 (97%) | 11 (3%)  | 0        | 100         | 100 |
| 46  | l     | 359/363 (99%)  | 347 (97%) | 12 (3%)  | 0        | 100         | 100 |
| 47  | m     | 290/298 (97%)  | 283 (98%) | 7 (2%)   | 0        | 100         | 100 |
| 48  | n     | 152/176 (86%)  | 143 (94%) | 9 (6%)   | 0        | 100         | 100 |
| 49  | o     | 229/241 (95%)  | 222 (97%) | 7 (3%)   | 0        | 100         | 100 |
| 50  | p     | 229/262 (87%)  | 223 (97%) | 6 (3%)   | 0        | 100         | 100 |
| 51  | q     | 187/191 (98%)  | 181 (97%) | 6 (3%)   | 0        | 100         | 100 |
| 52  | r     | 216/220 (98%)  | 210 (97%) | 6 (3%)   | 0        | 100         | 100 |
| 53  | s     | 171/174 (98%)  | 164 (96%) | 7 (4%)   | 0        | 100         | 100 |
| 54  | t     | 193/202 (96%)  | 184 (95%) | 8 (4%)   | 1 (0%)   | 24          | 27  |
| 55  | u     | 128/131 (98%)  | 125 (98%) | 3 (2%)   | 0        | 100         | 100 |
| 56  | v     | 201/204 (98%)  | 196 (98%) | 5 (2%)   | 0        | 100         | 100 |
| 57  | w     | 197/200 (98%)  | 194 (98%) | 3 (2%)   | 0        | 100         | 100 |
| 58  | x     | 168/185 (91%)  | 163 (97%) | 5 (3%)   | 0        | 100         | 100 |
| 59  | y     | 186/186 (100%) | 179 (96%) | 7 (4%)   | 0        | 100         | 100 |
| 60  | z     | 179/190 (94%)  | 178 (99%) | 1 (1%)   | 0        | 100         | 100 |
| 61  | AA    | 133/136 (98%)  | 131 (98%) | 2 (2%)   | 0        | 100         | 100 |
| 62  | AB    | 146/149 (98%)  | 141 (97%) | 5 (3%)   | 0        | 100         | 100 |
| 63  | AC    | 59/63 (94%)    | 58 (98%)  | 1 (2%)   | 0        | 100         | 100 |
| 64  | AD    | 94/106 (89%)   | 93 (99%)  | 1 (1%)   | 0        | 100         | 100 |
| 65  | AE    | 106/112 (95%)  | 102 (96%) | 4 (4%)   | 0        | 100         | 100 |
| 66  | AF    | 124/131 (95%)  | 123 (99%) | 1 (1%)   | 0        | 100         | 100 |
| 67  | AG    | 107/107 (100%) | 105 (98%) | 2 (2%)   | 0        | 100         | 100 |
| 68  | AH    | 114/122 (93%)  | 112 (98%) | 2 (2%)   | 0        | 100         | 100 |
| 69  | AI    | 118/120 (98%)  | 113 (96%) | 5 (4%)   | 0        | 100         | 100 |
| 70  | AJ    | 96/99 (97%)    | 95 (99%)  | 1 (1%)   | 0        | 100         | 100 |
| 71  | AK    | 84/90 (93%)    | 83 (99%)  | 1 (1%)   | 0        | 100         | 100 |
| 72  | AL    | 76/78 (97%)    | 74 (97%)  | 2 (3%)   | 0        | 100         | 100 |
| 73  | AM    | 49/51 (96%)    | 48 (98%)  | 1 (2%)   | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Favoured    | Allowed  | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 74  | AN    | 51/52 (98%)       | 51 (100%)   | 0        | 0        | 100         | 100 |
| 75  | AO    | 23/25 (92%)       | 21 (91%)    | 1 (4%)   | 1 (4%)   | 2           | 1   |
| 76  | AP    | 103/106 (97%)     | 98 (95%)    | 5 (5%)   | 0        | 100         | 100 |
| 77  | AQ    | 89/92 (97%)       | 85 (96%)    | 4 (4%)   | 0        | 100         | 100 |
| All | All   | 10639/11747 (91%) | 10148 (95%) | 484 (4%) | 7 (0%)   | 49          | 59  |

All (7) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 27  | T     | 103 | ASN  |
| 42  | g     | 186 | CYS  |
| 27  | T     | 102 | ALA  |
| 54  | t     | 63  | VAL  |
| 23  | N     | 27  | ALA  |
| 75  | AO    | 3   | ASP  |
| 11  | B     | 68  | PRO  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 1   | 0     | 158/157 (101%) | 156 (99%)  | 2 (1%)   | 61          | 76  |
| 3   | 2     | 135/134 (101%) | 135 (100%) | 0        | 100         | 100 |
| 6   | 6     | 101/103 (98%)  | 101 (100%) | 0        | 100         | 100 |
| 7   | 7     | 56/127 (44%)   | 56 (100%)  | 0        | 100         | 100 |
| 8   | 8     | 107/121 (88%)  | 107 (100%) | 0        | 100         | 100 |
| 9   | 9     | 110/112 (98%)  | 110 (100%) | 0        | 100         | 100 |
| 11  | B     | 176/215 (82%)  | 176 (100%) | 0        | 100         | 100 |
| 12  | C     | 194/229 (85%)  | 194 (100%) | 0        | 100         | 100 |
| 13  | D     | 174/198 (88%)  | 174 (100%) | 0        | 100         | 100 |
| 14  | E     | 173/196 (88%)  | 173 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Rotameric  | Outliers | Percentiles |     |
|-----|-------|---------------|------------|----------|-------------|-----|
| 15  | F     | 218/220 (99%) | 218 (100%) | 0        | 100         | 100 |
| 16  | G     | 173/197 (88%) | 173 (100%) | 0        | 100         | 100 |
| 17  | H     | 195/204 (96%) | 195 (100%) | 0        | 100         | 100 |
| 18  | I     | 163/167 (98%) | 163 (100%) | 0        | 100         | 100 |
| 19  | J     | 157/160 (98%) | 157 (100%) | 0        | 100         | 100 |
| 20  | K     | 153/160 (96%) | 153 (100%) | 0        | 100         | 100 |
| 21  | L     | 87/104 (84%)  | 87 (100%)  | 0        | 100         | 100 |
| 22  | M     | 122/134 (91%) | 122 (100%) | 0        | 100         | 100 |
| 23  | N     | 60/123 (49%)  | 60 (100%)  | 0        | 100         | 100 |
| 24  | O     | 129/130 (99%) | 129 (100%) | 0        | 100         | 100 |
| 25  | P     | 96/101 (95%)  | 96 (100%)  | 0        | 100         | 100 |
| 26  | Q     | 99/121 (82%)  | 99 (100%)  | 0        | 100         | 100 |
| 27  | T     | 126/129 (98%) | 126 (100%) | 0        | 100         | 100 |
| 28  | R     | 115/116 (99%) | 115 (100%) | 0        | 100         | 100 |
| 29  | S     | 106/122 (87%) | 106 (100%) | 0        | 100         | 100 |
| 30  | U     | 113/117 (97%) | 113 (100%) | 0        | 100         | 100 |
| 31  | V     | 90/105 (86%)  | 90 (100%)  | 0        | 100         | 100 |
| 32  | W     | 71/71 (100%)  | 71 (100%)  | 0        | 100         | 100 |
| 33  | X     | 112/113 (99%) | 112 (100%) | 0        | 100         | 100 |
| 34  | Y     | 116/118 (98%) | 116 (100%) | 0        | 100         | 100 |
| 35  | Z     | 109/112 (97%) | 109 (100%) | 0        | 100         | 100 |
| 36  | a     | 64/85 (75%)   | 64 (100%)  | 0        | 100         | 100 |
| 37  | b     | 84/102 (82%)  | 84 (100%)  | 0        | 100         | 100 |
| 38  | c     | 72/73 (99%)   | 71 (99%)   | 1 (1%)   | 59          | 73  |
| 39  | d     | 54/58 (93%)   | 54 (100%)  | 0        | 100         | 100 |
| 40  | e     | 47/48 (98%)   | 47 (100%)  | 0        | 100         | 100 |
| 41  | f     | 50/54 (93%)   | 50 (100%)  | 0        | 100         | 100 |
| 42  | g     | 60/175 (34%)  | 60 (100%)  | 0        | 100         | 100 |
| 43  | h     | 199/263 (76%) | 198 (100%) | 1 (0%)   | 81          | 89  |
| 44  | j     | 191/194 (98%) | 189 (99%)  | 2 (1%)   | 68          | 81  |
| 45  | k     | 326/328 (99%) | 326 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 46  | l     | 290/292 (99%)  | 290 (100%) | 0        | 100         | 100 |
| 47  | m     | 247/252 (98%)  | 247 (100%) | 0        | 100         | 100 |
| 48  | n     | 135/154 (88%)  | 135 (100%) | 0        | 100         | 100 |
| 49  | o     | 195/204 (96%)  | 195 (100%) | 0        | 100         | 100 |
| 50  | p     | 193/216 (89%)  | 193 (100%) | 0        | 100         | 100 |
| 51  | q     | 168/170 (99%)  | 168 (100%) | 0        | 100         | 100 |
| 52  | r     | 185/186 (100%) | 185 (100%) | 0        | 100         | 100 |
| 53  | s     | 148/149 (99%)  | 148 (100%) | 0        | 100         | 100 |
| 54  | t     | 163/168 (97%)  | 163 (100%) | 0        | 100         | 100 |
| 55  | u     | 108/109 (99%)  | 108 (100%) | 0        | 100         | 100 |
| 56  | v     | 177/178 (99%)  | 177 (100%) | 0        | 100         | 100 |
| 57  | w     | 166/167 (99%)  | 166 (100%) | 0        | 100         | 100 |
| 58  | x     | 142/154 (92%)  | 142 (100%) | 0        | 100         | 100 |
| 59  | y     | 156/154 (101%) | 154 (99%)  | 2 (1%)   | 61          | 76  |
| 60  | z     | 148/153 (97%)  | 148 (100%) | 0        | 100         | 100 |
| 61  | AA    | 117/118 (99%)  | 117 (100%) | 0        | 100         | 100 |
| 62  | AB    | 120/121 (99%)  | 120 (100%) | 0        | 100         | 100 |
| 63  | AC    | 48/49 (98%)    | 46 (96%)   | 2 (4%)   | 26          | 35  |
| 64  | AD    | 81/90 (90%)    | 81 (100%)  | 0        | 100         | 100 |
| 65  | AE    | 97/100 (97%)   | 97 (100%)  | 0        | 100         | 100 |
| 66  | AF    | 111/115 (96%)  | 109 (98%)  | 2 (2%)   | 51          | 66  |
| 67  | AG    | 94/92 (102%)   | 94 (100%)  | 0        | 100         | 100 |
| 68  | AH    | 99/102 (97%)   | 99 (100%)  | 0        | 100         | 100 |
| 69  | AI    | 106/106 (100%) | 106 (100%) | 0        | 100         | 100 |
| 70  | AJ    | 78/79 (99%)    | 78 (100%)  | 0        | 100         | 100 |
| 71  | AK    | 70/73 (96%)    | 70 (100%)  | 0        | 100         | 100 |
| 72  | AL    | 69/69 (100%)   | 67 (97%)   | 2 (3%)   | 37          | 49  |
| 73  | AM    | 47/47 (100%)   | 47 (100%)  | 0        | 100         | 100 |
| 74  | AN    | 48/47 (102%)   | 48 (100%)  | 0        | 100         | 100 |
| 75  | AO    | 24/24 (100%)   | 24 (100%)  | 0        | 100         | 100 |
| 76  | AP    | 90/89 (101%)   | 90 (100%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Rotameric   | Outliers | Percentiles |     |
|-----|-------|-----------------|-------------|----------|-------------|-----|
| 77  | AQ    | 72/73 (99%)     | 72 (100%)   | 0        | 100         | 100 |
| All | All   | 9133/9896 (92%) | 9119 (100%) | 14 (0%)  | 87          | 94  |

All (14) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | 0     | 138[A] | GLN  |
| 1   | 0     | 138[B] | GLN  |
| 38  | c     | 42     | ASN  |
| 43  | h     | 122    | GLN  |
| 44  | j     | 70[A]  | LYS  |
| 44  | j     | 70[B]  | LYS  |
| 59  | y     | 31[A]  | LYS  |
| 59  | y     | 31[B]  | LYS  |
| 63  | AC    | 14[A]  | ARG  |
| 63  | AC    | 14[B]  | ARG  |
| 66  | AF    | 17[A]  | LYS  |
| 66  | AF    | 17[B]  | LYS  |
| 72  | AL    | 30[A]  | LYS  |
| 72  | AL    | 30[B]  | LYS  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (93) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | 2     | 16  | GLN  |
| 9   | 9     | 86  | GLN  |
| 11  | B     | 30  | GLN  |
| 12  | C     | 124 | ASN  |
| 13  | D     | 84  | GLN  |
| 13  | D     | 89  | GLN  |
| 13  | D     | 145 | GLN  |
| 15  | F     | 36  | HIS  |
| 15  | F     | 50  | ASN  |
| 15  | F     | 188 | ASN  |
| 16  | G     | 224 | ASN  |
| 17  | H     | 56  | ASN  |
| 17  | H     | 69  | HIS  |
| 18  | I     | 27  | GLN  |
| 18  | I     | 38  | GLN  |
| 20  | K     | 131 | GLN  |
| 20  | K     | 176 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 22  | M     | 14  | GLN  |
| 24  | O     | 49  | GLN  |
| 25  | P     | 19  | ASN  |
| 27  | T     | 19  | ASN  |
| 27  | T     | 75  | ASN  |
| 27  | T     | 89  | GLN  |
| 27  | T     | 137 | HIS  |
| 28  | R     | 93  | GLN  |
| 28  | R     | 138 | GLN  |
| 29  | S     | 42  | GLN  |
| 29  | S     | 56  | HIS  |
| 30  | U     | 12  | GLN  |
| 31  | V     | 19  | HIS  |
| 31  | V     | 46  | GLN  |
| 34  | Y     | 63  | GLN  |
| 35  | Z     | 15  | ASN  |
| 35  | Z     | 29  | HIS  |
| 38  | c     | 38  | GLN  |
| 38  | c     | 51  | GLN  |
| 41  | f     | 31  | GLN  |
| 43  | h     | 311 | GLN  |
| 44  | j     | 140 | ASN  |
| 44  | j     | 205 | ASN  |
| 44  | j     | 211 | HIS  |
| 45  | k     | 173 | GLN  |
| 45  | k     | 182 | GLN  |
| 45  | k     | 231 | HIS  |
| 46  | l     | 111 | ASN  |
| 46  | l     | 312 | HIS  |
| 46  | l     | 321 | ASN  |
| 46  | l     | 356 | GLN  |
| 47  | m     | 13  | HIS  |
| 47  | m     | 94  | ASN  |
| 48  | n     | 10  | GLN  |
| 48  | n     | 71  | ASN  |
| 49  | o     | 50  | GLN  |
| 49  | o     | 91  | ASN  |
| 49  | o     | 108 | GLN  |
| 50  | p     | 222 | ASN  |
| 51  | q     | 77  | ASN  |
| 51  | q     | 96  | HIS  |
| 51  | q     | 109 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 52  | r     | 59  | GLN  |
| 52  | r     | 73  | ASN  |
| 54  | t     | 66  | ASN  |
| 54  | t     | 102 | GLN  |
| 54  | t     | 177 | ASN  |
| 55  | u     | 112 | GLN  |
| 56  | v     | 32  | GLN  |
| 56  | v     | 91  | GLN  |
| 58  | x     | 10  | ASN  |
| 58  | x     | 55  | GLN  |
| 58  | x     | 137 | ASN  |
| 59  | y     | 9   | GLN  |
| 59  | y     | 58  | ASN  |
| 59  | y     | 158 | HIS  |
| 60  | z     | 7   | GLN  |
| 60  | z     | 47  | ASN  |
| 60  | z     | 130 | ASN  |
| 60  | z     | 166 | ASN  |
| 61  | AA    | 29  | HIS  |
| 62  | AB    | 14  | ASN  |
| 62  | AB    | 49  | HIS  |
| 64  | AD    | 77  | ASN  |
| 65  | AE    | 14  | ASN  |
| 65  | AE    | 20  | HIS  |
| 66  | AF    | 21  | HIS  |
| 66  | AF    | 53  | GLN  |
| 68  | AH    | 69  | HIS  |
| 69  | AI    | 16  | GLN  |
| 69  | AI    | 59  | ASN  |
| 69  | AI    | 99  | GLN  |
| 72  | AL    | 40  | GLN  |
| 72  | AL    | 66  | GLN  |
| 73  | AM    | 17  | GLN  |
| 73  | AM    | 25  | GLN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 10  | A     | 1685/1787 (94%) | 379 (22%)         | 25 (1%)         |
| 2   | 1     | 3060/3359 (91%) | 455 (14%)         | 27 (0%)         |
| 4   | 3     | 120/121 (99%)   | 10 (8%)           | 0               |

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| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 5   | 4     | 155/158 (98%)   | 23 (14%)          | 2 (1%)          |
| 78  | AT    | 75/77 (97%)     | 21 (28%)          | 0               |
| 78  | PT    | 75/77 (97%)     | 16 (21%)          | 0               |
| 79  | MR    | 10/39 (25%)     | 0                 | 0               |
| All | All   | 5180/5618 (92%) | 904 (17%)         | 54 (1%)         |

All (904) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | 1     | 13  | U    |
| 2   | 1     | 24  | U    |
| 2   | 1     | 25  | A    |
| 2   | 1     | 29  | G    |
| 2   | 1     | 39  | A    |
| 2   | 1     | 42  | A    |
| 2   | 1     | 48  | A    |
| 2   | 1     | 58  | G    |
| 2   | 1     | 59  | A    |
| 2   | 1     | 64  | A    |
| 2   | 1     | 65  | A    |
| 2   | 1     | 91  | G    |
| 2   | 1     | 98  | A    |
| 2   | 1     | 104 | C    |
| 2   | 1     | 108 | A    |
| 2   | 1     | 109 | G    |
| 2   | 1     | 110 | C    |
| 2   | 1     | 121 | A    |
| 2   | 1     | 135 | G    |
| 2   | 1     | 155 | A    |
| 2   | 1     | 156 | A    |
| 2   | 1     | 163 | A    |
| 2   | 1     | 164 | U    |
| 2   | 1     | 172 | C    |
| 2   | 1     | 173 | C    |
| 2   | 1     | 175 | G    |
| 2   | 1     | 176 | G    |
| 2   | 1     | 189 | U    |
| 2   | 1     | 190 | U    |
| 2   | 1     | 199 | C    |
| 2   | 1     | 205 | G    |
| 2   | 1     | 209 | C    |
| 2   | 1     | 212 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | 1     | 217 | G    |
| 2   | 1     | 218 | A    |
| 2   | 1     | 219 | G    |
| 2   | 1     | 230 | G    |
| 2   | 1     | 239 | A    |
| 2   | 1     | 240 | C    |
| 2   | 1     | 243 | G    |
| 2   | 1     | 248 | U    |
| 2   | 1     | 249 | G    |
| 2   | 1     | 250 | U    |
| 2   | 1     | 253 | A    |
| 2   | 1     | 269 | G    |
| 2   | 1     | 286 | U    |
| 2   | 1     | 295 | A    |
| 2   | 1     | 305 | U    |
| 2   | 1     | 311 | C    |
| 2   | 1     | 323 | A    |
| 2   | 1     | 329 | U    |
| 2   | 1     | 339 | C    |
| 2   | 1     | 349 | A    |
| 2   | 1     | 350 | C    |
| 2   | 1     | 376 | G    |
| 2   | 1     | 377 | A    |
| 2   | 1     | 398 | A    |
| 2   | 1     | 401 | U    |
| 2   | 1     | 402 | A    |
| 2   | 1     | 403 | C    |
| 2   | 1     | 420 | G    |
| 2   | 1     | 421 | G    |
| 2   | 1     | 422 | A    |
| 2   | 1     | 438 | A    |
| 2   | 1     | 439 | C    |
| 2   | 1     | 506 | A    |
| 2   | 1     | 517 | A    |
| 2   | 1     | 531 | G    |
| 2   | 1     | 539 | G    |
| 2   | 1     | 540 | C    |
| 2   | 1     | 542 | U    |
| 2   | 1     | 543 | C    |
| 2   | 1     | 544 | U    |
| 2   | 1     | 545 | G    |
| 2   | 1     | 546 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | 1     | 555 | A    |
| 2   | 1     | 556 | U    |
| 2   | 1     | 557 | A    |
| 2   | 1     | 564 | G    |
| 2   | 1     | 576 | A    |
| 2   | 1     | 577 | G    |
| 2   | 1     | 590 | A    |
| 2   | 1     | 598 | U    |
| 2   | 1     | 600 | U    |
| 2   | 1     | 601 | U    |
| 2   | 1     | 602 | A    |
| 2   | 1     | 609 | A    |
| 2   | 1     | 618 | U    |
| 2   | 1     | 619 | A    |
| 2   | 1     | 620 | A    |
| 2   | 1     | 621 | U    |
| 2   | 1     | 634 | C    |
| 2   | 1     | 647 | A    |
| 2   | 1     | 658 | A    |
| 2   | 1     | 675 | A    |
| 2   | 1     | 679 | U    |
| 2   | 1     | 689 | A    |
| 2   | 1     | 703 | A    |
| 2   | 1     | 710 | G    |
| 2   | 1     | 713 | A    |
| 2   | 1     | 730 | A    |
| 2   | 1     | 731 | U    |
| 2   | 1     | 732 | U    |
| 2   | 1     | 733 | A    |
| 2   | 1     | 763 | U    |
| 2   | 1     | 772 | U    |
| 2   | 1     | 773 | U    |
| 2   | 1     | 776 | A    |
| 2   | 1     | 777 | G    |
| 2   | 1     | 781 | G    |
| 2   | 1     | 802 | A    |
| 2   | 1     | 813 | A    |
| 2   | 1     | 826 | A    |
| 2   | 1     | 845 | C    |
| 2   | 1     | 857 | C    |
| 2   | 1     | 870 | U    |
| 2   | 1     | 875 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | 1     | 886  | C    |
| 2   | 1     | 892  | A    |
| 2   | 1     | 903  | G    |
| 2   | 1     | 904  | G    |
| 2   | 1     | 910  | A    |
| 2   | 1     | 912  | G    |
| 2   | 1     | 913  | A    |
| 2   | 1     | 919  | C    |
| 2   | 1     | 920  | G    |
| 2   | 1     | 921  | A    |
| 2   | 1     | 933  | G    |
| 2   | 1     | 940  | C    |
| 2   | 1     | 955  | C    |
| 2   | 1     | 956  | U    |
| 2   | 1     | 976  | A    |
| 2   | 1     | 990  | G    |
| 2   | 1     | 998  | A    |
| 2   | 1     | 1006 | G    |
| 2   | 1     | 1011 | C    |
| 2   | 1     | 1012 | U    |
| 2   | 1     | 1013 | U    |
| 2   | 1     | 1014 | G    |
| 2   | 1     | 1016 | G    |
| 2   | 1     | 1030 | U    |
| 2   | 1     | 1032 | A    |
| 2   | 1     | 1043 | A    |
| 2   | 1     | 1045 | C    |
| 2   | 1     | 1060 | A    |
| 2   | 1     | 1061 | A    |
| 2   | 1     | 1068 | G    |
| 2   | 1     | 1077 | U    |
| 2   | 1     | 1078 | U    |
| 2   | 1     | 1090 | A    |
| 2   | 1     | 1092 | U    |
| 2   | 1     | 1093 | G    |
| 2   | 1     | 1094 | A    |
| 2   | 1     | 1099 | A    |
| 2   | 1     | 1100 | G    |
| 2   | 1     | 1113 | G    |
| 2   | 1     | 1127 | G    |
| 2   | 1     | 1149 | A    |
| 2   | 1     | 1155 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | 1     | 1176 | A    |
| 2   | 1     | 1177 | U    |
| 2   | 1     | 1178 | G    |
| 2   | 1     | 1188 | C    |
| 2   | 1     | 1189 | A    |
| 2   | 1     | 1192 | C    |
| 2   | 1     | 1197 | C    |
| 2   | 1     | 1205 | G    |
| 2   | 1     | 1215 | C    |
| 2   | 1     | 1217 | A    |
| 2   | 1     | 1283 | A    |
| 2   | 1     | 1303 | G    |
| 2   | 1     | 1304 | A    |
| 2   | 1     | 1305 | U    |
| 2   | 1     | 1326 | A    |
| 2   | 1     | 1339 | A    |
| 2   | 1     | 1344 | U    |
| 2   | 1     | 1346 | U    |
| 2   | 1     | 1347 | U    |
| 2   | 1     | 1348 | U    |
| 2   | 1     | 1349 | U    |
| 2   | 1     | 1382 | A    |
| 2   | 1     | 1395 | U    |
| 2   | 1     | 1415 | A    |
| 2   | 1     | 1421 | U    |
| 2   | 1     | 1430 | G    |
| 2   | 1     | 1433 | C    |
| 2   | 1     | 1442 | A    |
| 2   | 1     | 1446 | G    |
| 2   | 1     | 1465 | C    |
| 2   | 1     | 1471 | A    |
| 2   | 1     | 1477 | A    |
| 2   | 1     | 1483 | G    |
| 2   | 1     | 1504 | C    |
| 2   | 1     | 1523 | C    |
| 2   | 1     | 1532 | G    |
| 2   | 1     | 1535 | A    |
| 2   | 1     | 1550 | U    |
| 2   | 1     | 1551 | U    |
| 2   | 1     | 1552 | C    |
| 2   | 1     | 1556 | G    |
| 2   | 1     | 1558 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | 1     | 1560 | U    |
| 2   | 1     | 1562 | G    |
| 2   | 1     | 1563 | A    |
| 2   | 1     | 1565 | U    |
| 2   | 1     | 1566 | U    |
| 2   | 1     | 1567 | U    |
| 2   | 1     | 1568 | U    |
| 2   | 1     | 1571 | G    |
| 2   | 1     | 1572 | G    |
| 2   | 1     | 1574 | C    |
| 2   | 1     | 1576 | A    |
| 2   | 1     | 1585 | A    |
| 2   | 1     | 1589 | A    |
| 2   | 1     | 1601 | A    |
| 2   | 1     | 1625 | U    |
| 2   | 1     | 1635 | C    |
| 2   | 1     | 1638 | A    |
| 2   | 1     | 1639 | A    |
| 2   | 1     | 1641 | U    |
| 2   | 1     | 1653 | C    |
| 2   | 1     | 1679 | A    |
| 2   | 1     | 1720 | U    |
| 2   | 1     | 1721 | C    |
| 2   | 1     | 1732 | G    |
| 2   | 1     | 1746 | A    |
| 2   | 1     | 1747 | G    |
| 2   | 1     | 1759 | U    |
| 2   | 1     | 1761 | U    |
| 2   | 1     | 1762 | G    |
| 2   | 1     | 1763 | C    |
| 2   | 1     | 1776 | G    |
| 2   | 1     | 1792 | G    |
| 2   | 1     | 1793 | A    |
| 2   | 1     | 1804 | G    |
| 2   | 1     | 1809 | A    |
| 2   | 1     | 1810 | A    |
| 2   | 1     | 1812 | A    |
| 2   | 1     | 1813 | G    |
| 2   | 1     | 1814 | U    |
| 2   | 1     | 1815 | U    |
| 2   | 1     | 1816 | U    |
| 2   | 1     | 1817 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | 1     | 1835 | A    |
| 2   | 1     | 1838 | A    |
| 2   | 1     | 1842 | C    |
| 2   | 1     | 1845 | C    |
| 2   | 1     | 1862 | C    |
| 2   | 1     | 1874 | G    |
| 2   | 1     | 1875 | A    |
| 2   | 1     | 1876 | U    |
| 2   | 1     | 1882 | A    |
| 2   | 1     | 1902 | G    |
| 2   | 1     | 2070 | A    |
| 2   | 1     | 2072 | C    |
| 2   | 1     | 2073 | G    |
| 2   | 1     | 2078 | A    |
| 2   | 1     | 2089 | G    |
| 2   | 1     | 2090 | U    |
| 2   | 1     | 2091 | A    |
| 2   | 1     | 2092 | C    |
| 2   | 1     | 2099 | G    |
| 2   | 1     | 2100 | G    |
| 2   | 1     | 2109 | A    |
| 2   | 1     | 2118 | U    |
| 2   | 1     | 2122 | A    |
| 2   | 1     | 2136 | A    |
| 2   | 1     | 2147 | G    |
| 2   | 1     | 2149 | G    |
| 2   | 1     | 2185 | A    |
| 2   | 1     | 2186 | A    |
| 2   | 1     | 2187 | U    |
| 2   | 1     | 2188 | G    |
| 2   | 1     | 2203 | U    |
| 2   | 1     | 2222 | A    |
| 2   | 1     | 2227 | G    |
| 2   | 1     | 2235 | C    |
| 2   | 1     | 2250 | G    |
| 2   | 1     | 2251 | G    |
| 2   | 1     | 2259 | A    |
| 2   | 1     | 2260 | U    |
| 2   | 1     | 2276 | U    |
| 2   | 1     | 2285 | G    |
| 2   | 1     | 2288 | U    |
| 2   | 1     | 2291 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | 1     | 2292 | U    |
| 2   | 1     | 2293 | G    |
| 2   | 1     | 2312 | U    |
| 2   | 1     | 2313 | G    |
| 2   | 1     | 2314 | U    |
| 2   | 1     | 2341 | A    |
| 2   | 1     | 2351 | A    |
| 2   | 1     | 2352 | C    |
| 2   | 1     | 2353 | G    |
| 2   | 1     | 2363 | G    |
| 2   | 1     | 2366 | U    |
| 2   | 1     | 2371 | G    |
| 2   | 1     | 2372 | G    |
| 2   | 1     | 2375 | A    |
| 2   | 1     | 2380 | A    |
| 2   | 1     | 2381 | G    |
| 2   | 1     | 2382 | A    |
| 2   | 1     | 2389 | U    |
| 2   | 1     | 2390 | G    |
| 2   | 1     | 2397 | A    |
| 2   | 1     | 2413 | G    |
| 2   | 1     | 2420 | G    |
| 2   | 1     | 2421 | A    |
| 2   | 1     | 2422 | C    |
| 2   | 1     | 2492 | U    |
| 2   | 1     | 2493 | A    |
| 2   | 1     | 2500 | G    |
| 2   | 1     | 2509 | C    |
| 2   | 1     | 2511 | G    |
| 2   | 1     | 2516 | U    |
| 2   | 1     | 2517 | C    |
| 2   | 1     | 2518 | A    |
| 2   | 1     | 2519 | A    |
| 2   | 1     | 2520 | A    |
| 2   | 1     | 2526 | C    |
| 2   | 1     | 2527 | G    |
| 2   | 1     | 2529 | U    |
| 2   | 1     | 2530 | C    |
| 2   | 1     | 2532 | A    |
| 2   | 1     | 2533 | G    |
| 2   | 1     | 2536 | U    |
| 2   | 1     | 2537 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | 1     | 2538 | A    |
| 2   | 1     | 2545 | C    |
| 2   | 1     | 2546 | U    |
| 2   | 1     | 2547 | G    |
| 2   | 1     | 2557 | G    |
| 2   | 1     | 2565 | A    |
| 2   | 1     | 2566 | C    |
| 2   | 1     | 2578 | G    |
| 2   | 1     | 2579 | G    |
| 2   | 1     | 2586 | G    |
| 2   | 1     | 2624 | U    |
| 2   | 1     | 2628 | A    |
| 2   | 1     | 2646 | A    |
| 2   | 1     | 2649 | G    |
| 2   | 1     | 2650 | A    |
| 2   | 1     | 2661 | A    |
| 2   | 1     | 2662 | G    |
| 2   | 1     | 2663 | A    |
| 2   | 1     | 2666 | A    |
| 2   | 1     | 2676 | A    |
| 2   | 1     | 2686 | G    |
| 2   | 1     | 2691 | U    |
| 2   | 1     | 2700 | G    |
| 2   | 1     | 2701 | U    |
| 2   | 1     | 2725 | G    |
| 2   | 1     | 2727 | C    |
| 2   | 1     | 2734 | A    |
| 2   | 1     | 2744 | C    |
| 2   | 1     | 2749 | G    |
| 2   | 1     | 2750 | G    |
| 2   | 1     | 2768 | G    |
| 2   | 1     | 2771 | A    |
| 2   | 1     | 2772 | G    |
| 2   | 1     | 2773 | A    |
| 2   | 1     | 2782 | C    |
| 2   | 1     | 2786 | G    |
| 2   | 1     | 2789 | A    |
| 2   | 1     | 2790 | U    |
| 2   | 1     | 2791 | A    |
| 2   | 1     | 2814 | U    |
| 2   | 1     | 2815 | U    |
| 2   | 1     | 2816 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | 1     | 2817 | A    |
| 2   | 1     | 2821 | C    |
| 2   | 1     | 2833 | U    |
| 2   | 1     | 2839 | C    |
| 2   | 1     | 2843 | G    |
| 2   | 1     | 2844 | A    |
| 2   | 1     | 2847 | U    |
| 2   | 1     | 2859 | A    |
| 2   | 1     | 2871 | C    |
| 2   | 1     | 2886 | G    |
| 2   | 1     | 2895 | U    |
| 2   | 1     | 2907 | U    |
| 2   | 1     | 2908 | A    |
| 2   | 1     | 2914 | C    |
| 2   | 1     | 2919 | G    |
| 2   | 1     | 2943 | A    |
| 2   | 1     | 2955 | C    |
| 2   | 1     | 2962 | G    |
| 2   | 1     | 2969 | G    |
| 2   | 1     | 2984 | A    |
| 2   | 1     | 3028 | U    |
| 2   | 1     | 3031 | G    |
| 2   | 1     | 3050 | A    |
| 2   | 1     | 3051 | C    |
| 2   | 1     | 3052 | G    |
| 2   | 1     | 3058 | A    |
| 2   | 1     | 3064 | C    |
| 2   | 1     | 3065 | C    |
| 2   | 1     | 3073 | G    |
| 2   | 1     | 3076 | U    |
| 2   | 1     | 3094 | A    |
| 2   | 1     | 3101 | A    |
| 2   | 1     | 3102 | A    |
| 2   | 1     | 3103 | U    |
| 2   | 1     | 3114 | A    |
| 2   | 1     | 3115 | C    |
| 2   | 1     | 3125 | U    |
| 2   | 1     | 3143 | G    |
| 2   | 1     | 3144 | A    |
| 2   | 1     | 3145 | U    |
| 2   | 1     | 3146 | G    |
| 2   | 1     | 3149 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | 1     | 3151 | C    |
| 2   | 1     | 3157 | A    |
| 2   | 1     | 3163 | U    |
| 2   | 1     | 3164 | U    |
| 2   | 1     | 3165 | U    |
| 2   | 1     | 3171 | C    |
| 2   | 1     | 3172 | U    |
| 2   | 1     | 3175 | A    |
| 2   | 1     | 3182 | C    |
| 2   | 1     | 3183 | A    |
| 2   | 1     | 3184 | G    |
| 2   | 1     | 3194 | G    |
| 2   | 1     | 3208 | A    |
| 2   | 1     | 3210 | A    |
| 2   | 1     | 3211 | G    |
| 2   | 1     | 3212 | G    |
| 2   | 1     | 3214 | U    |
| 2   | 1     | 3217 | G    |
| 2   | 1     | 3224 | U    |
| 2   | 1     | 3228 | G    |
| 2   | 1     | 3235 | A    |
| 2   | 1     | 3238 | A    |
| 2   | 1     | 3241 | G    |
| 2   | 1     | 3246 | C    |
| 2   | 1     | 3252 | C    |
| 2   | 1     | 3259 | A    |
| 2   | 1     | 3260 | A    |
| 2   | 1     | 3269 | C    |
| 2   | 1     | 3278 | U    |
| 2   | 1     | 3281 | A    |
| 2   | 1     | 3284 | U    |
| 2   | 1     | 3306 | U    |
| 2   | 1     | 3310 | G    |
| 2   | 1     | 3314 | C    |
| 2   | 1     | 3316 | U    |
| 2   | 1     | 3318 | G    |
| 2   | 1     | 3319 | U    |
| 2   | 1     | 3320 | U    |
| 2   | 1     | 3321 | G    |
| 2   | 1     | 3334 | G    |
| 2   | 1     | 3343 | C    |
| 2   | 1     | 3347 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | 1     | 3351 | G    |
| 2   | 1     | 3361 | U    |
| 4   | 3     | 7    | G    |
| 4   | 3     | 22   | A    |
| 4   | 3     | 23   | A    |
| 4   | 3     | 42   | A    |
| 4   | 3     | 54   | U    |
| 4   | 3     | 65   | G    |
| 4   | 3     | 73   | C    |
| 4   | 3     | 76   | A    |
| 4   | 3     | 102  | A    |
| 4   | 3     | 112  | G    |
| 5   | 4     | 34   | U    |
| 5   | 4     | 35   | C    |
| 5   | 4     | 59   | A    |
| 5   | 4     | 62   | C    |
| 5   | 4     | 63   | G    |
| 5   | 4     | 80   | U    |
| 5   | 4     | 81   | A    |
| 5   | 4     | 84   | C    |
| 5   | 4     | 86   | U    |
| 5   | 4     | 87   | G    |
| 5   | 4     | 92   | A    |
| 5   | 4     | 95   | G    |
| 5   | 4     | 102  | U    |
| 5   | 4     | 104  | A    |
| 5   | 4     | 106  | C    |
| 5   | 4     | 111  | A    |
| 5   | 4     | 113  | U    |
| 5   | 4     | 125  | U    |
| 5   | 4     | 126  | A    |
| 5   | 4     | 128  | U    |
| 5   | 4     | 129  | C    |
| 5   | 4     | 148  | G    |
| 5   | 4     | 152  | G    |
| 10  | A     | 25   | C    |
| 10  | A     | 26   | A    |
| 10  | A     | 27   | U    |
| 10  | A     | 34   | G    |
| 10  | A     | 42   | G    |
| 10  | A     | 45   | U    |
| 10  | A     | 47   | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10  | A     | 57  | G    |
| 10  | A     | 59  | C    |
| 10  | A     | 66  | U    |
| 10  | A     | 68  | A    |
| 10  | A     | 73  | U    |
| 10  | A     | 74  | U    |
| 10  | A     | 75  | U    |
| 10  | A     | 77  | U    |
| 10  | A     | 78  | A    |
| 10  | A     | 81  | G    |
| 10  | A     | 84  | A    |
| 10  | A     | 100 | A    |
| 10  | A     | 104 | A    |
| 10  | A     | 111 | U    |
| 10  | A     | 114 | C    |
| 10  | A     | 123 | G    |
| 10  | A     | 127 | G    |
| 10  | A     | 129 | A    |
| 10  | A     | 138 | C    |
| 10  | A     | 139 | U    |
| 10  | A     | 142 | G    |
| 10  | A     | 143 | A    |
| 10  | A     | 151 | G    |
| 10  | A     | 152 | G    |
| 10  | A     | 159 | U    |
| 10  | A     | 168 | U    |
| 10  | A     | 173 | G    |
| 10  | A     | 174 | C    |
| 10  | A     | 176 | U    |
| 10  | A     | 177 | A    |
| 10  | A     | 179 | A    |
| 10  | A     | 192 | U    |
| 10  | A     | 193 | G    |
| 10  | A     | 197 | G    |
| 10  | A     | 199 | G    |
| 10  | A     | 200 | A    |
| 10  | A     | 202 | G    |
| 10  | A     | 211 | A    |
| 10  | A     | 213 | A    |
| 10  | A     | 214 | U    |
| 10  | A     | 215 | A    |
| 10  | A     | 216 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10  | A     | 217 | A    |
| 10  | A     | 218 | A    |
| 10  | A     | 219 | A    |
| 10  | A     | 255 | A    |
| 10  | A     | 259 | U    |
| 10  | A     | 260 | U    |
| 10  | A     | 261 | C    |
| 10  | A     | 262 | G    |
| 10  | A     | 269 | A    |
| 10  | A     | 270 | U    |
| 10  | A     | 274 | C    |
| 10  | A     | 276 | U    |
| 10  | A     | 278 | U    |
| 10  | A     | 279 | G    |
| 10  | A     | 282 | G    |
| 10  | A     | 283 | G    |
| 10  | A     | 285 | G    |
| 10  | A     | 288 | G    |
| 10  | A     | 297 | A    |
| 10  | A     | 299 | A    |
| 10  | A     | 307 | C    |
| 10  | A     | 312 | C    |
| 10  | A     | 314 | A    |
| 10  | A     | 318 | U    |
| 10  | A     | 320 | G    |
| 10  | A     | 335 | G    |
| 10  | A     | 336 | C    |
| 10  | A     | 350 | A    |
| 10  | A     | 357 | A    |
| 10  | A     | 358 | A    |
| 10  | A     | 359 | C    |
| 10  | A     | 398 | A    |
| 10  | A     | 400 | C    |
| 10  | A     | 402 | G    |
| 10  | A     | 416 | G    |
| 10  | A     | 421 | G    |
| 10  | A     | 422 | C    |
| 10  | A     | 423 | A    |
| 10  | A     | 424 | G    |
| 10  | A     | 432 | G    |
| 10  | A     | 435 | A    |
| 10  | A     | 437 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10  | A     | 442 | C    |
| 10  | A     | 458 | A    |
| 10  | A     | 462 | A    |
| 10  | A     | 466 | A    |
| 10  | A     | 475 | A    |
| 10  | A     | 480 | U    |
| 10  | A     | 482 | C    |
| 10  | A     | 483 | A    |
| 10  | A     | 501 | G    |
| 10  | A     | 502 | U    |
| 10  | A     | 503 | A    |
| 10  | A     | 504 | A    |
| 10  | A     | 505 | U    |
| 10  | A     | 506 | U    |
| 10  | A     | 509 | A    |
| 10  | A     | 512 | G    |
| 10  | A     | 513 | A    |
| 10  | A     | 515 | U    |
| 10  | A     | 517 | C    |
| 10  | A     | 525 | A    |
| 10  | A     | 530 | U    |
| 10  | A     | 534 | C    |
| 10  | A     | 537 | G    |
| 10  | A     | 539 | A    |
| 10  | A     | 540 | A    |
| 10  | A     | 553 | A    |
| 10  | A     | 554 | A    |
| 10  | A     | 555 | G    |
| 10  | A     | 556 | U    |
| 10  | A     | 557 | C    |
| 10  | A     | 563 | C    |
| 10  | A     | 566 | G    |
| 10  | A     | 576 | U    |
| 10  | A     | 577 | A    |
| 10  | A     | 580 | U    |
| 10  | A     | 581 | C    |
| 10  | A     | 592 | A    |
| 10  | A     | 593 | G    |
| 10  | A     | 604 | A    |
| 10  | A     | 609 | U    |
| 10  | A     | 617 | A    |
| 10  | A     | 618 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10  | A     | 620 | A    |
| 10  | A     | 621 | A    |
| 10  | A     | 622 | G    |
| 10  | A     | 651 | C    |
| 10  | A     | 652 | C    |
| 10  | A     | 653 | G    |
| 10  | A     | 654 | G    |
| 10  | A     | 676 | G    |
| 10  | A     | 682 | A    |
| 10  | A     | 689 | C    |
| 10  | A     | 690 | C    |
| 10  | A     | 691 | U    |
| 10  | A     | 693 | U    |
| 10  | A     | 695 | C    |
| 10  | A     | 696 | U    |
| 10  | A     | 697 | U    |
| 10  | A     | 698 | C    |
| 10  | A     | 700 | G    |
| 10  | A     | 701 | G    |
| 10  | A     | 722 | A    |
| 10  | A     | 723 | G    |
| 10  | A     | 724 | G    |
| 10  | A     | 730 | U    |
| 10  | A     | 736 | G    |
| 10  | A     | 740 | A    |
| 10  | A     | 741 | A    |
| 10  | A     | 750 | G    |
| 10  | A     | 751 | U    |
| 10  | A     | 756 | A    |
| 10  | A     | 759 | A    |
| 10  | A     | 760 | G    |
| 10  | A     | 763 | C    |
| 10  | A     | 764 | U    |
| 10  | A     | 765 | U    |
| 10  | A     | 766 | U    |
| 10  | A     | 767 | G    |
| 10  | A     | 771 | G    |
| 10  | A     | 773 | A    |
| 10  | A     | 775 | A    |
| 10  | A     | 778 | U    |
| 10  | A     | 779 | U    |
| 10  | A     | 785 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10  | A     | 796 | A    |
| 10  | A     | 798 | A    |
| 10  | A     | 802 | C    |
| 10  | A     | 805 | U    |
| 10  | A     | 815 | U    |
| 10  | A     | 816 | U    |
| 10  | A     | 818 | U    |
| 10  | A     | 819 | G    |
| 10  | A     | 820 | U    |
| 10  | A     | 821 | U    |
| 10  | A     | 822 | G    |
| 10  | A     | 823 | G    |
| 10  | A     | 824 | U    |
| 10  | A     | 828 | U    |
| 10  | A     | 829 | A    |
| 10  | A     | 834 | C    |
| 10  | A     | 837 | C    |
| 10  | A     | 840 | A    |
| 10  | A     | 841 | A    |
| 10  | A     | 842 | U    |
| 10  | A     | 847 | A    |
| 10  | A     | 848 | A    |
| 10  | A     | 858 | U    |
| 10  | A     | 869 | A    |
| 10  | A     | 877 | G    |
| 10  | A     | 879 | U    |
| 10  | A     | 881 | U    |
| 10  | A     | 897 | U    |
| 10  | A     | 898 | G    |
| 10  | A     | 899 | G    |
| 10  | A     | 900 | A    |
| 10  | A     | 910 | G    |
| 10  | A     | 911 | A    |
| 10  | A     | 918 | A    |
| 10  | A     | 920 | U    |
| 10  | A     | 945 | U    |
| 10  | A     | 951 | A    |
| 10  | A     | 969 | G    |
| 10  | A     | 973 | A    |
| 10  | A     | 977 | A    |
| 10  | A     | 988 | A    |
| 10  | A     | 989 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 10  | A     | 1011 | A    |
| 10  | A     | 1013 | C    |
| 10  | A     | 1016 | U    |
| 10  | A     | 1025 | G    |
| 10  | A     | 1036 | U    |
| 10  | A     | 1037 | U    |
| 10  | A     | 1038 | G    |
| 10  | A     | 1039 | U    |
| 10  | A     | 1042 | U    |
| 10  | A     | 1043 | U    |
| 10  | A     | 1044 | U    |
| 10  | A     | 1046 | A    |
| 10  | A     | 1047 | U    |
| 10  | A     | 1056 | U    |
| 10  | A     | 1058 | G    |
| 10  | A     | 1059 | G    |
| 10  | A     | 1061 | A    |
| 10  | A     | 1068 | G    |
| 10  | A     | 1077 | A    |
| 10  | A     | 1081 | C    |
| 10  | A     | 1085 | G    |
| 10  | A     | 1123 | A    |
| 10  | A     | 1128 | A    |
| 10  | A     | 1135 | G    |
| 10  | A     | 1143 | C    |
| 10  | A     | 1145 | A    |
| 10  | A     | 1148 | A    |
| 10  | A     | 1152 | G    |
| 10  | A     | 1168 | A    |
| 10  | A     | 1169 | A    |
| 10  | A     | 1170 | U    |
| 10  | A     | 1171 | U    |
| 10  | A     | 1179 | A    |
| 10  | A     | 1181 | A    |
| 10  | A     | 1184 | G    |
| 10  | A     | 1185 | G    |
| 10  | A     | 1186 | G    |
| 10  | A     | 1187 | A    |
| 10  | A     | 1193 | A    |
| 10  | A     | 1202 | A    |
| 10  | A     | 1203 | G    |
| 10  | A     | 1213 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 10  | A     | 1214 | G    |
| 10  | A     | 1215 | A    |
| 10  | A     | 1220 | C    |
| 10  | A     | 1228 | G    |
| 10  | A     | 1229 | A    |
| 10  | A     | 1230 | G    |
| 10  | A     | 1231 | C    |
| 10  | A     | 1235 | U    |
| 10  | A     | 1236 | U    |
| 10  | A     | 1237 | C    |
| 10  | A     | 1244 | U    |
| 10  | A     | 1270 | U    |
| 10  | A     | 1284 | G    |
| 10  | A     | 1298 | A    |
| 10  | A     | 1299 | U    |
| 10  | A     | 1300 | U    |
| 10  | A     | 1306 | A    |
| 10  | A     | 1310 | A    |
| 10  | A     | 1325 | U    |
| 10  | A     | 1326 | A    |
| 10  | A     | 1336 | G    |
| 10  | A     | 1337 | C    |
| 10  | A     | 1342 | A    |
| 10  | A     | 1343 | G    |
| 10  | A     | 1345 | A    |
| 10  | A     | 1346 | U    |
| 10  | A     | 1348 | U    |
| 10  | A     | 1349 | G    |
| 10  | A     | 1352 | G    |
| 10  | A     | 1356 | U    |
| 10  | A     | 1357 | A    |
| 10  | A     | 1358 | G    |
| 10  | A     | 1359 | U    |
| 10  | A     | 1360 | C    |
| 10  | A     | 1369 | G    |
| 10  | A     | 1370 | A    |
| 10  | A     | 1376 | U    |
| 10  | A     | 1382 | U    |
| 10  | A     | 1384 | U    |
| 10  | A     | 1385 | C    |
| 10  | A     | 1388 | G    |
| 10  | A     | 1392 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 10  | A     | 1398 | G    |
| 10  | A     | 1399 | U    |
| 10  | A     | 1400 | U    |
| 10  | A     | 1401 | U    |
| 10  | A     | 1405 | G    |
| 10  | A     | 1413 | A    |
| 10  | A     | 1414 | G    |
| 10  | A     | 1422 | A    |
| 10  | A     | 1431 | G    |
| 10  | A     | 1432 | A    |
| 10  | A     | 1433 | C    |
| 10  | A     | 1445 | C    |
| 10  | A     | 1446 | A    |
| 10  | A     | 1447 | C    |
| 10  | A     | 1457 | A    |
| 10  | A     | 1461 | A    |
| 10  | A     | 1462 | C    |
| 10  | A     | 1463 | G    |
| 10  | A     | 1467 | C    |
| 10  | A     | 1476 | A    |
| 10  | A     | 1477 | U    |
| 10  | A     | 1478 | A    |
| 10  | A     | 1479 | A    |
| 10  | A     | 1480 | G    |
| 10  | A     | 1481 | C    |
| 10  | A     | 1483 | U    |
| 10  | A     | 1485 | G    |
| 10  | A     | 1486 | G    |
| 10  | A     | 1491 | G    |
| 10  | A     | 1502 | A    |
| 10  | A     | 1503 | A    |
| 10  | A     | 1508 | G    |
| 10  | A     | 1510 | G    |
| 10  | A     | 1511 | A    |
| 10  | A     | 1523 | G    |
| 10  | A     | 1525 | U    |
| 10  | A     | 1529 | G    |
| 10  | A     | 1530 | A    |
| 10  | A     | 1537 | A    |
| 10  | A     | 1544 | U    |
| 10  | A     | 1546 | G    |
| 10  | A     | 1556 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 10  | A     | 1561 | G    |
| 10  | A     | 1571 | G    |
| 10  | A     | 1577 | G    |
| 10  | A     | 1580 | A    |
| 10  | A     | 1582 | U    |
| 10  | A     | 1584 | A    |
| 10  | A     | 1588 | G    |
| 10  | A     | 1590 | U    |
| 10  | A     | 1602 | C    |
| 10  | A     | 1603 | G    |
| 10  | A     | 1609 | G    |
| 10  | A     | 1621 | C    |
| 10  | A     | 1644 | U    |
| 10  | A     | 1645 | G    |
| 10  | A     | 1665 | C    |
| 10  | A     | 1667 | G    |
| 10  | A     | 1672 | G    |
| 10  | A     | 1673 | U    |
| 10  | A     | 1674 | U    |
| 10  | A     | 1677 | G    |
| 10  | A     | 1700 | G    |
| 10  | A     | 1702 | A    |
| 10  | A     | 1742 | A    |
| 10  | A     | 1744 | G    |
| 10  | A     | 1747 | G    |
| 10  | A     | 1749 | A    |
| 10  | A     | 1753 | A    |
| 10  | A     | 1756 | U    |
| 10  | A     | 1765 | G    |
| 10  | A     | 1767 | G    |
| 10  | A     | 1770 | C    |
| 10  | A     | 1779 | G    |
| 10  | A     | 1780 | G    |
| 10  | A     | 1781 | A    |
| 10  | A     | 1782 | U    |
| 10  | A     | 1783 | C    |
| 78  | PT    | 3    | C    |
| 78  | PT    | 6    | G    |
| 78  | PT    | 9    | G    |
| 78  | PT    | 11   | A    |
| 78  | PT    | 16   | C    |
| 78  | PT    | 17   | C    |

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| Mol | Chain | Res   | Type |
|-----|-------|-------|------|
| 78  | PT    | 18(A) | U    |
| 78  | PT    | 20    | G    |
| 78  | PT    | 21    | U    |
| 78  | PT    | 22    | A    |
| 78  | PT    | 48    | U    |
| 78  | PT    | 49    | C    |
| 78  | PT    | 50    | G    |
| 78  | PT    | 71    | G    |
| 78  | PT    | 75    | C    |
| 78  | PT    | 77    | A    |
| 78  | AT    | 4     | G    |
| 78  | AT    | 5     | G    |
| 78  | AT    | 6     | G    |
| 78  | AT    | 7     | G    |
| 78  | AT    | 8     | U    |
| 78  | AT    | 9     | G    |
| 78  | AT    | 11    | A    |
| 78  | AT    | 13    | C    |
| 78  | AT    | 16    | C    |
| 78  | AT    | 18(A) | U    |
| 78  | AT    | 19    | G    |
| 78  | AT    | 21    | U    |
| 78  | AT    | 22    | A    |
| 78  | AT    | 31    | G    |
| 78  | AT    | 45    | A    |
| 78  | AT    | 50    | G    |
| 78  | AT    | 59    | A    |
| 78  | AT    | 70    | C    |
| 78  | AT    | 73    | A    |
| 78  | AT    | 75    | C    |
| 78  | AT    | 77    | A    |

All (54) RNA pucker outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | 1     | 172  | C    |
| 2   | 1     | 538  | G    |
| 2   | 1     | 563  | U    |
| 2   | 1     | 586  | G    |
| 2   | 1     | 601  | U    |
| 2   | 1     | 912  | G    |
| 2   | 1     | 1012 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 2   | 1     | 1060 | A    |
| 2   | 1     | 1099 | A    |
| 2   | 1     | 1346 | U    |
| 2   | 1     | 1347 | U    |
| 2   | 1     | 1559 | C    |
| 2   | 1     | 1762 | G    |
| 2   | 1     | 1815 | U    |
| 2   | 1     | 2090 | U    |
| 2   | 1     | 2515 | G    |
| 2   | 1     | 2519 | A    |
| 2   | 1     | 2557 | G    |
| 2   | 1     | 2789 | A    |
| 2   | 1     | 2790 | U    |
| 2   | 1     | 3093 | U    |
| 2   | 1     | 3163 | U    |
| 2   | 1     | 3193 | C    |
| 2   | 1     | 3234 | U    |
| 2   | 1     | 3240 | U    |
| 2   | 1     | 3315 | C    |
| 2   | 1     | 3317 | U    |
| 5   | 4     | 79   | A    |
| 5   | 4     | 85   | G    |
| 10  | A     | 137  | A    |
| 10  | A     | 151  | G    |
| 10  | A     | 176  | U    |
| 10  | A     | 214  | U    |
| 10  | A     | 218  | A    |
| 10  | A     | 259  | U    |
| 10  | A     | 415  | A    |
| 10  | A     | 503  | A    |
| 10  | A     | 504  | A    |
| 10  | A     | 505  | U    |
| 10  | A     | 514  | G    |
| 10  | A     | 529  | C    |
| 10  | A     | 553  | A    |
| 10  | A     | 740  | A    |
| 10  | A     | 763  | C    |
| 10  | A     | 765  | U    |
| 10  | A     | 820  | U    |
| 10  | A     | 876  | A    |
| 10  | A     | 1168 | A    |
| 10  | A     | 1369 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 10  | A     | 1398 | G    |
| 10  | A     | 1479 | A    |
| 10  | A     | 1555 | C    |
| 10  | A     | 1579 | A    |
| 10  | A     | 1581 | G    |

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

6 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 | $\# Z  > 2$ |
| 2   | OMC  | 1     | 2808 | 2    | 19,22,23     | 2.89 | 8 (42%)     | 25,31,34    | 1.22 | 3 (12%)     |
| 6   | MLZ  | 6     | 110  | 6    | 8,9,10       | 0.72 | 0           | 4,9,11      | 0.87 | 0           |
| 25  | IAS  | P     | 119  | 25   | 6,7,8        | 1.11 | 0           | 4,8,10      | 1.44 | 1 (25%)     |
| 2   | OMG  | 1     | 2765 | 2    | 23,26,27     | 2.30 | 9 (39%)     | 32,38,41    | 1.88 | 9 (28%)     |
| 76  | MLZ  | AP    | 55   | 76   | 8,9,10       | 0.69 | 0           | 4,9,11      | 0.81 | 0           |
| 76  | MLZ  | AP    | 40   | 76   | 8,9,10       | 0.68 | 0           | 4,9,11      | 0.89 | 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   |
|-----|------|-------|------|------|---------|-----------|---------|
| 2   | OMC  | 1     | 2808 | 2    | -       | 2/9/27/28 | 0/2/2/2 |
| 6   | MLZ  | 6     | 110  | 6    | -       | 3/7/8/10  | -       |
| 25  | IAS  | P     | 119  | 25   | -       | 4/5/6/8   | -       |
| 2   | OMG  | 1     | 2765 | 2    | -       | 1/9/27/28 | 0/3/3/3 |
| 76  | MLZ  | AP    | 55   | 76   | -       | 1/7/8/10  | -       |
| 76  | MLZ  | AP    | 40   | 76   | -       | 0/7/8/10  | -       |

All (17) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 2   | 1     | 2765 | OMG  | C4-N3 | 6.13  | 1.48        | 1.34     |
| 2   | 1     | 2808 | OMC  | C2-N3 | 6.04  | 1.48        | 1.36     |
| 2   | 1     | 2808 | OMC  | C6-C5 | 5.76  | 1.48        | 1.35     |
| 2   | 1     | 2765 | OMG  | C2-N3 | 5.27  | 1.46        | 1.33     |
| 2   | 1     | 2808 | OMC  | C2-N1 | 4.72  | 1.50        | 1.40     |
| 2   | 1     | 2808 | OMC  | C4-N4 | 4.55  | 1.44        | 1.33     |
| 2   | 1     | 2808 | OMC  | C4-N3 | 4.54  | 1.43        | 1.34     |
| 2   | 1     | 2765 | OMG  | C2-N2 | 3.81  | 1.43        | 1.34     |
| 2   | 1     | 2808 | OMC  | O2-C2 | -3.17 | 1.17        | 1.23     |
| 2   | 1     | 2765 | OMG  | O6-C6 | -3.07 | 1.17        | 1.23     |
| 2   | 1     | 2808 | OMC  | C6-N1 | 2.95  | 1.45        | 1.38     |
| 2   | 1     | 2765 | OMG  | C5-N7 | -2.88 | 1.33        | 1.39     |
| 2   | 1     | 2765 | OMG  | C4-N9 | -2.34 | 1.32        | 1.38     |
| 2   | 1     | 2765 | OMG  | C5-C6 | 2.29  | 1.53        | 1.44     |
| 2   | 1     | 2765 | OMG  | C2-N1 | 2.25  | 1.43        | 1.37     |
| 2   | 1     | 2808 | OMC  | C5-C4 | 2.23  | 1.48        | 1.42     |
| 2   | 1     | 2765 | OMG  | C6-N1 | 2.18  | 1.42        | 1.38     |

All (13) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 2   | 1     | 2765 | OMG  | C5-C4-N3   | -4.65 | 120.99      | 128.39   |
| 2   | 1     | 2765 | OMG  | C2-N3-C4   | 4.45  | 119.97      | 112.30   |
| 2   | 1     | 2765 | OMG  | N9-C8-N7   | -3.47 | 106.97      | 113.40   |
| 2   | 1     | 2808 | OMC  | O2-C2-N3   | -3.40 | 116.97      | 122.33   |
| 2   | 1     | 2765 | OMG  | C2-N1-C6   | -2.87 | 119.90      | 125.11   |
| 2   | 1     | 2765 | OMG  | C5-C6-N1   | 2.71  | 120.15      | 113.25   |
| 2   | 1     | 2765 | OMG  | N9-C4-N3   | 2.63  | 131.21      | 125.95   |
| 2   | 1     | 2765 | OMG  | O6-C6-C5   | -2.36 | 120.31      | 126.53   |
| 2   | 1     | 2808 | OMC  | C1'-N1-C2  | 2.32  | 123.57      | 118.44   |
| 2   | 1     | 2765 | OMG  | C8-N7-C5   | 2.30  | 108.35      | 104.26   |
| 2   | 1     | 2808 | OMC  | C6-C5-C4   | 2.23  | 121.18      | 117.53   |
| 2   | 1     | 2765 | OMG  | C2'-C1'-N9 | -2.10 | 110.26      | 114.24   |
| 25  | P     | 119  | IAS  | OD2-CG-CB  | 2.08  | 120.46      | 114.00   |

There are no chirality outliers.

All (11) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms         |
|-----|-------|------|------|---------------|
| 2   | 1     | 2808 | OMC  | O4'-C1'-N1-C2 |
| 2   | 1     | 2808 | OMC  | O4'-C1'-N1-C6 |
| 6   | 6     | 110  | MLZ  | CD-CE-NZ-CM   |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 25  | P     | 119  | IAS  | C-CA-CB-CG      |
| 25  | P     | 119  | IAS  | N-CA-CB-CG      |
| 76  | AP    | 55   | MLZ  | CA-CB-CG-CD     |
| 6   | 6     | 110  | MLZ  | C-CA-CB-CG      |
| 25  | P     | 119  | IAS  | CA-CB-CG-OD2    |
| 2   | 1     | 2765 | OMG  | C3'-C2'-O2'-CM2 |
| 25  | P     | 119  | IAS  | CA-CB-CG-OD1    |
| 6   | 6     | 110  | MLZ  | CE-CD-CG-CB     |

There are no ring outliers.

2 monomers are involved in 3 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 2   | 1     | 2808 | OMC  | 2       | 0            |
| 25  | P     | 119  | IAS  | 1       | 0            |

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 25 ligands modelled in this entry, 7 are monoatomic - leaving 18 for Mogul analysis.

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 | $\# Z  > 2$ |
| 80  | SPK  | 1     | 3401 | -    | 13,13,13     | 0.37 | 0           | 12,12,12    | 0.78 | 0           |
| 81  | GET  | 1     | 3404 | -    | 35,36,36     | 0.80 | 1 (2%)      | 43,55,55    | 0.74 | 2 (4%)      |
| 81  | GET  | 1     | 3412 | -    | 35,36,36     | 1.49 | 1 (2%)      | 43,55,55    | 0.74 | 0           |
| 81  | GET  | A     | 1801 | -    | 35,36,36     | 0.46 | 0           | 43,55,55    | 0.72 | 1 (2%)      |
| 81  | GET  | A     | 1804 | -    | 35,36,36     | 1.10 | 1 (2%)      | 43,55,55    | 0.82 | 1 (2%)      |
| 81  | GET  | 1     | 3407 | -    | 35,36,36     | 0.46 | 0           | 43,55,55    | 0.88 | 3 (6%)      |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 81  | GET  | 1     | 3406 | -    | 35,36,36     | 1.19 | 1 (2%)   | 43,55,55    | 0.83 | 2 (4%)   |
| 81  | GET  | 1     | 3409 | -    | 35,36,36     | 0.50 | 0        | 43,55,55    | 0.78 | 2 (4%)   |
| 81  | GET  | 1     | 3410 | -    | 35,36,36     | 0.94 | 1 (2%)   | 43,55,55    | 0.88 | 3 (6%)   |
| 81  | GET  | AT    | 101  | -    | 35,36,36     | 0.90 | 1 (2%)   | 43,55,55    | 0.53 | 0        |
| 81  | GET  | 1     | 3411 | -    | 35,36,36     | 0.55 | 0        | 43,55,55    | 0.94 | 3 (6%)   |
| 81  | GET  | A     | 1803 | -    | 35,36,36     | 0.63 | 1 (2%)   | 43,55,55    | 0.70 | 1 (2%)   |
| 81  | GET  | 1     | 3405 | -    | 35,36,36     | 0.69 | 1 (2%)   | 43,55,55    | 0.78 | 1 (2%)   |
| 81  | GET  | A     | 1802 | -    | 35,36,36     | 0.98 | 1 (2%)   | 43,55,55    | 0.86 | 1 (2%)   |
| 81  | GET  | 1     | 3408 | -    | 35,36,36     | 0.85 | 1 (2%)   | 43,55,55    | 0.66 | 1 (2%)   |
| 81  | GET  | 1     | 3413 | -    | 35,36,36     | 0.79 | 1 (2%)   | 43,55,55    | 0.93 | 3 (6%)   |
| 81  | GET  | 1     | 3403 | -    | 35,36,36     | 0.64 | 1 (2%)   | 43,55,55    | 0.95 | 2 (4%)   |
| 81  | GET  | 1     | 3402 | -    | 35,36,36     | 0.87 | 1 (2%)   | 43,55,55    | 0.62 | 1 (2%)   |

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   |
|-----|------|-------|------|------|---------|-------------|---------|
| 80  | SPK  | 1     | 3401 | -    | -       | 4/11/11/11  | -       |
| 81  | GET  | 1     | 3404 | -    | -       | 2/13/74/74  | 1/3/3/3 |
| 81  | GET  | 1     | 3412 | -    | -       | 1/13/74/74  | 0/3/3/3 |
| 81  | GET  | A     | 1801 | -    | -       | 1/13/74/74  | 0/3/3/3 |
| 81  | GET  | A     | 1804 | -    | -       | 10/13/74/74 | 1/3/3/3 |
| 81  | GET  | 1     | 3407 | -    | -       | 1/13/74/74  | 0/3/3/3 |
| 81  | GET  | 1     | 3406 | -    | -       | 2/13/74/74  | 0/3/3/3 |
| 81  | GET  | 1     | 3409 | -    | -       | 3/13/74/74  | 0/3/3/3 |
| 81  | GET  | 1     | 3410 | -    | -       | 1/13/74/74  | 0/3/3/3 |
| 81  | GET  | AT    | 101  | -    | -       | 2/13/74/74  | 1/3/3/3 |
| 81  | GET  | 1     | 3411 | -    | -       | 6/13/74/74  | 1/3/3/3 |
| 81  | GET  | A     | 1803 | -    | -       | 1/13/74/74  | 0/3/3/3 |
| 81  | GET  | 1     | 3405 | -    | -       | 1/13/74/74  | 0/3/3/3 |
| 81  | GET  | A     | 1802 | -    | -       | 2/13/74/74  | 1/3/3/3 |
| 81  | GET  | 1     | 3408 | -    | -       | 1/13/74/74  | 0/3/3/3 |
| 81  | GET  | 1     | 3413 | -    | -       | 7/13/74/74  | 0/3/3/3 |
| 81  | GET  | 1     | 3403 | -    | -       | 6/13/74/74  | 1/3/3/3 |
| 81  | GET  | 1     | 3402 | -    | -       | 1/13/74/74  | 0/3/3/3 |

All (13) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 81  | 1     | 3412 | GET  | C33-N33 | 8.33  | 1.56        | 1.45     |
| 81  | 1     | 3406 | GET  | C33-N33 | 6.54  | 1.53        | 1.45     |
| 81  | A     | 1804 | GET  | C33-N33 | 5.71  | 1.52        | 1.45     |
| 81  | A     | 1802 | GET  | C33-N33 | 5.19  | 1.52        | 1.45     |
| 81  | 1     | 3410 | GET  | C33-N33 | 4.98  | 1.51        | 1.45     |
| 81  | AT    | 101  | GET  | C33-N33 | 4.52  | 1.51        | 1.45     |
| 81  | 1     | 3402 | GET  | C33-N33 | 4.44  | 1.51        | 1.45     |
| 81  | 1     | 3408 | GET  | C33-N33 | -4.43 | 1.40        | 1.45     |
| 81  | 1     | 3413 | GET  | C33-N33 | 3.88  | 1.50        | 1.45     |
| 81  | 1     | 3404 | GET  | C33-N33 | 3.77  | 1.50        | 1.45     |
| 81  | 1     | 3405 | GET  | C33-N33 | -3.20 | 1.41        | 1.45     |
| 81  | A     | 1803 | GET  | C33-N33 | 2.67  | 1.49        | 1.45     |
| 81  | 1     | 3403 | GET  | C11-C21 | -2.08 | 1.48        | 1.52     |

All (27) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 81  | A     | 1802 | GET  | O11-C11-C21 | 4.37  | 115.22      | 108.08   |
| 81  | 1     | 3406 | GET  | O11-C11-C21 | 3.96  | 114.56      | 108.08   |
| 81  | 1     | 3410 | GET  | O11-C11-C21 | 3.89  | 114.44      | 108.08   |
| 81  | 1     | 3405 | GET  | O11-C11-C21 | 3.60  | 113.97      | 108.08   |
| 81  | 1     | 3408 | GET  | O11-C11-C21 | 3.40  | 113.64      | 108.08   |
| 81  | 1     | 3407 | GET  | O62-C62-C12 | -3.23 | 101.48      | 109.18   |
| 81  | A     | 1803 | GET  | O11-C11-C21 | 3.15  | 113.23      | 108.08   |
| 81  | 1     | 3407 | GET  | O11-C11-C21 | 3.08  | 113.11      | 108.08   |
| 81  | 1     | 3403 | GET  | O11-C11-C21 | 2.85  | 112.74      | 108.08   |
| 81  | 1     | 3413 | GET  | O11-C42-C32 | -2.77 | 102.58      | 109.18   |
| 81  | 1     | 3402 | GET  | O11-C11-C21 | 2.73  | 112.54      | 108.08   |
| 81  | 1     | 3409 | GET  | O11-C11-C21 | 2.67  | 112.45      | 108.08   |
| 81  | A     | 1801 | GET  | O11-C11-C21 | 2.37  | 111.95      | 108.08   |
| 81  | 1     | 3411 | GET  | O11-C42-C52 | -2.36 | 101.23      | 107.23   |
| 81  | 1     | 3413 | GET  | O11-C42-C52 | 2.35  | 113.20      | 107.23   |
| 81  | 1     | 3403 | GET  | O62-C62-C52 | -2.34 | 101.28      | 107.23   |
| 81  | A     | 1804 | GET  | C32-C22-C12 | 2.30  | 114.97      | 111.02   |
| 81  | 1     | 3407 | GET  | C32-C22-C12 | -2.27 | 107.12      | 111.02   |
| 81  | 1     | 3404 | GET  | O62-C62-C12 | -2.25 | 103.80      | 109.18   |
| 81  | 1     | 3406 | GET  | O62-C62-C12 | -2.22 | 103.89      | 109.18   |
| 81  | 1     | 3404 | GET  | O11-C11-C21 | 2.11  | 111.53      | 108.08   |
| 81  | 1     | 3410 | GET  | O62-C62-C12 | -2.08 | 104.22      | 109.18   |
| 81  | 1     | 3413 | GET  | O11-C11-C21 | 2.08  | 111.47      | 108.08   |
| 81  | 1     | 3411 | GET  | C32-C22-C12 | -2.06 | 107.49      | 111.02   |
| 81  | 1     | 3411 | GET  | O11-C11-C21 | 2.06  | 111.44      | 108.08   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 81  | 1     | 3409 | GET  | C53-O53-C13 | 2.02  | 114.65      | 111.53   |
| 81  | 1     | 3410 | GET  | C32-C22-C12 | -2.02 | 107.55      | 111.02   |

There are no chirality outliers.

All (52) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 81  | 1     | 3402 | GET  | C23-C33-N33-C93 |
| 81  | 1     | 3403 | GET  | C21-C11-O11-C42 |
| 81  | 1     | 3403 | GET  | C41-C51-C61-O61 |
| 81  | 1     | 3403 | GET  | C41-C51-C61-C71 |
| 81  | 1     | 3403 | GET  | O51-C51-C61-C71 |
| 81  | 1     | 3404 | GET  | C23-C33-N33-C93 |
| 81  | 1     | 3405 | GET  | C23-C33-N33-C93 |
| 81  | 1     | 3407 | GET  | C23-C33-N33-C93 |
| 81  | 1     | 3409 | GET  | C23-C33-N33-C93 |
| 81  | 1     | 3410 | GET  | C23-C33-N33-C93 |
| 81  | 1     | 3411 | GET  | C21-C11-O11-C42 |
| 81  | 1     | 3411 | GET  | O51-C51-C61-O61 |
| 81  | 1     | 3411 | GET  | C23-C33-N33-C93 |
| 81  | 1     | 3412 | GET  | C23-C33-N33-C93 |
| 81  | 1     | 3413 | GET  | C41-C51-C61-O61 |
| 81  | 1     | 3413 | GET  | C41-C51-C61-C71 |
| 81  | 1     | 3413 | GET  | O51-C51-C61-O61 |
| 81  | 1     | 3413 | GET  | O51-C51-C61-C71 |
| 81  | 1     | 3413 | GET  | C23-C33-N33-C93 |
| 81  | A     | 1801 | GET  | C23-C33-N33-C93 |
| 81  | A     | 1802 | GET  | C23-C33-N33-C93 |
| 81  | A     | 1803 | GET  | C23-C33-N33-C93 |
| 81  | A     | 1804 | GET  | C32-C42-O11-C11 |
| 81  | A     | 1804 | GET  | C41-C51-C61-O61 |
| 81  | A     | 1804 | GET  | C41-C51-C61-C71 |
| 81  | A     | 1804 | GET  | O51-C51-C61-C71 |
| 81  | A     | 1804 | GET  | C23-C33-N33-C93 |
| 81  | 1     | 3413 | GET  | C52-C42-O11-C11 |
| 80  | 1     | 3401 | SPK  | C7-C8-C9-N10    |
| 81  | AT    | 101  | GET  | O51-C11-O11-C42 |
| 80  | 1     | 3401 | SPK  | C3-C4-N5-C6     |
| 81  | 1     | 3411 | GET  | O51-C51-C61-C71 |
| 81  | 1     | 3403 | GET  | O51-C11-O11-C42 |
| 81  | A     | 1804 | GET  | O53-C13-O62-C62 |
| 81  | A     | 1804 | GET  | C52-C62-O62-C13 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 81  | 1     | 3409 | GET  | O51-C11-O11-C42 |
| 81  | A     | 1804 | GET  | O51-C51-C61-O61 |
| 80  | 1     | 3401 | SPK  | C6-C7-C8-C9     |
| 81  | 1     | 3411 | GET  | C41-C51-C61-O61 |
| 81  | 1     | 3411 | GET  | C41-C51-C61-C71 |
| 81  | 1     | 3409 | GET  | C52-C42-O11-C11 |
| 80  | 1     | 3401 | SPK  | C7-C6-N5-C4     |
| 81  | 1     | 3403 | GET  | O51-C51-C61-O61 |
| 81  | A     | 1804 | GET  | C52-C42-O11-C11 |
| 81  | 1     | 3406 | GET  | C23-C33-N33-C93 |
| 81  | 1     | 3408 | GET  | C23-C33-N33-C93 |
| 81  | AT    | 101  | GET  | C23-C33-N33-C93 |
| 81  | A     | 1804 | GET  | C23-C13-O62-C62 |
| 81  | 1     | 3404 | GET  | O53-C13-O62-C62 |
| 81  | 1     | 3406 | GET  | O51-C11-O11-C42 |
| 81  | 1     | 3413 | GET  | C32-C42-O11-C11 |
| 81  | A     | 1802 | GET  | O51-C51-C61-O61 |

All (6) ring outliers are listed below:

| Mol | Chain | Res  | Type | Atoms                   |
|-----|-------|------|------|-------------------------|
| 81  | 1     | 3403 | GET  | C11-C21-C31-C41-C51-O51 |
| 81  | 1     | 3404 | GET  | C13-C23-C33-C43-C53-O53 |
| 81  | A     | 1802 | GET  | C11-C21-C31-C41-C51-O51 |
| 81  | A     | 1804 | GET  | C11-C21-C31-C41-C51-O51 |
| 81  | AT    | 101  | GET  | C11-C21-C31-C41-C51-O51 |
| 81  | 1     | 3411 | GET  | C11-C21-C31-C41-C51-O51 |

15 monomers are involved in 30 short contacts:

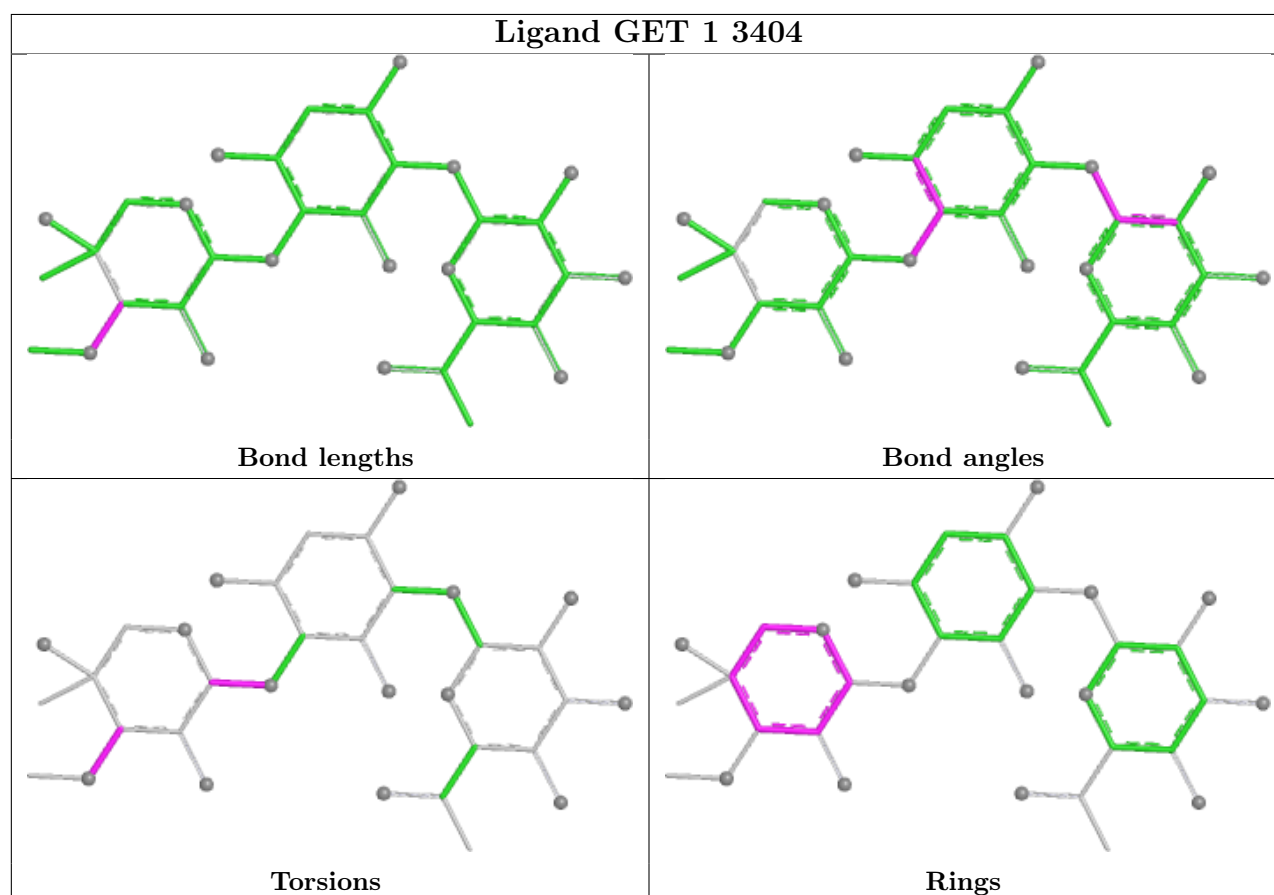
| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 80  | 1     | 3401 | SPK  | 1       | 0            |
| 81  | 1     | 3404 | GET  | 3       | 0            |
| 81  | 1     | 3412 | GET  | 3       | 0            |
| 81  | A     | 1801 | GET  | 3       | 0            |
| 81  | A     | 1804 | GET  | 3       | 0            |
| 81  | 1     | 3407 | GET  | 2       | 0            |
| 81  | 1     | 3406 | GET  | 2       | 0            |
| 81  | 1     | 3409 | GET  | 1       | 0            |
| 81  | 1     | 3410 | GET  | 1       | 0            |
| 81  | AT    | 101  | GET  | 1       | 0            |
| 81  | 1     | 3405 | GET  | 1       | 0            |

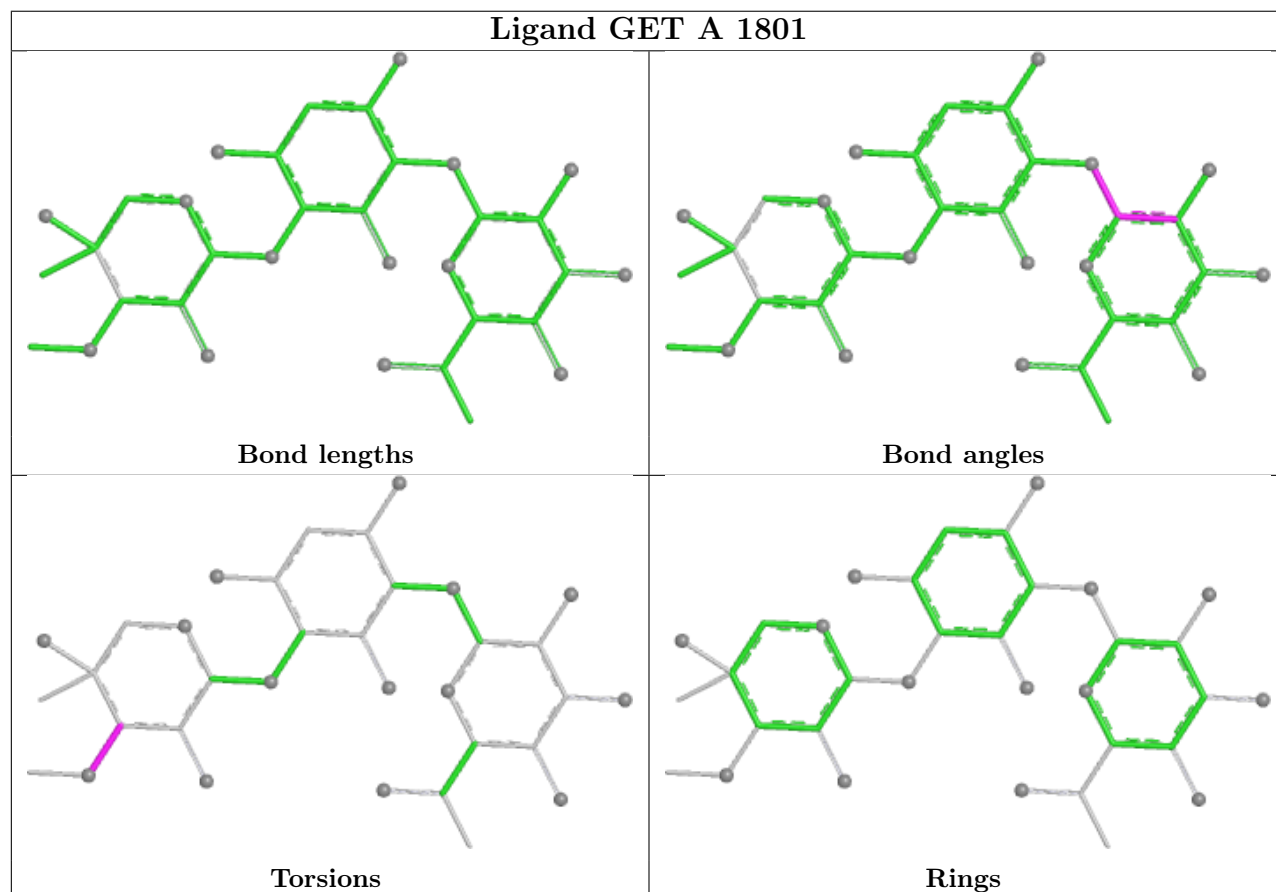
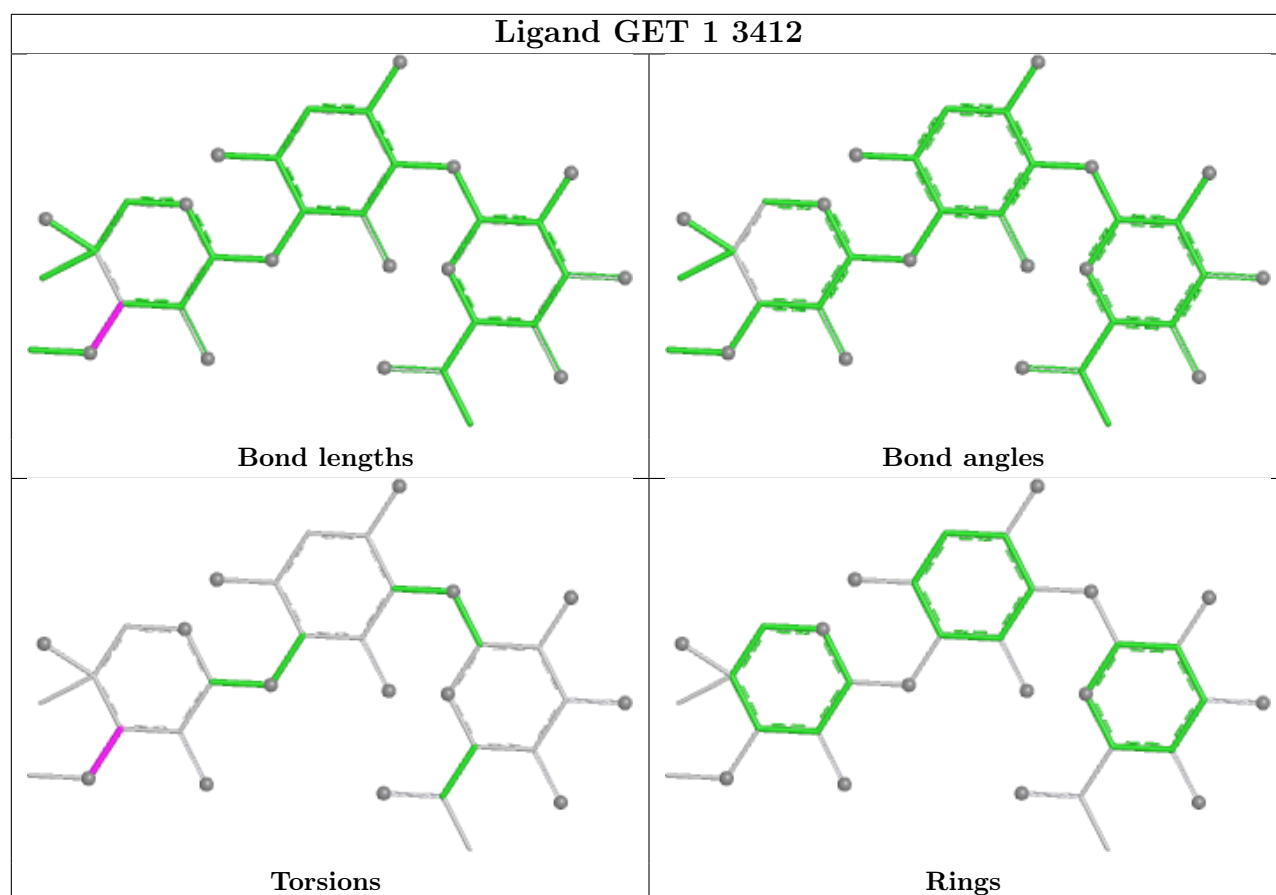
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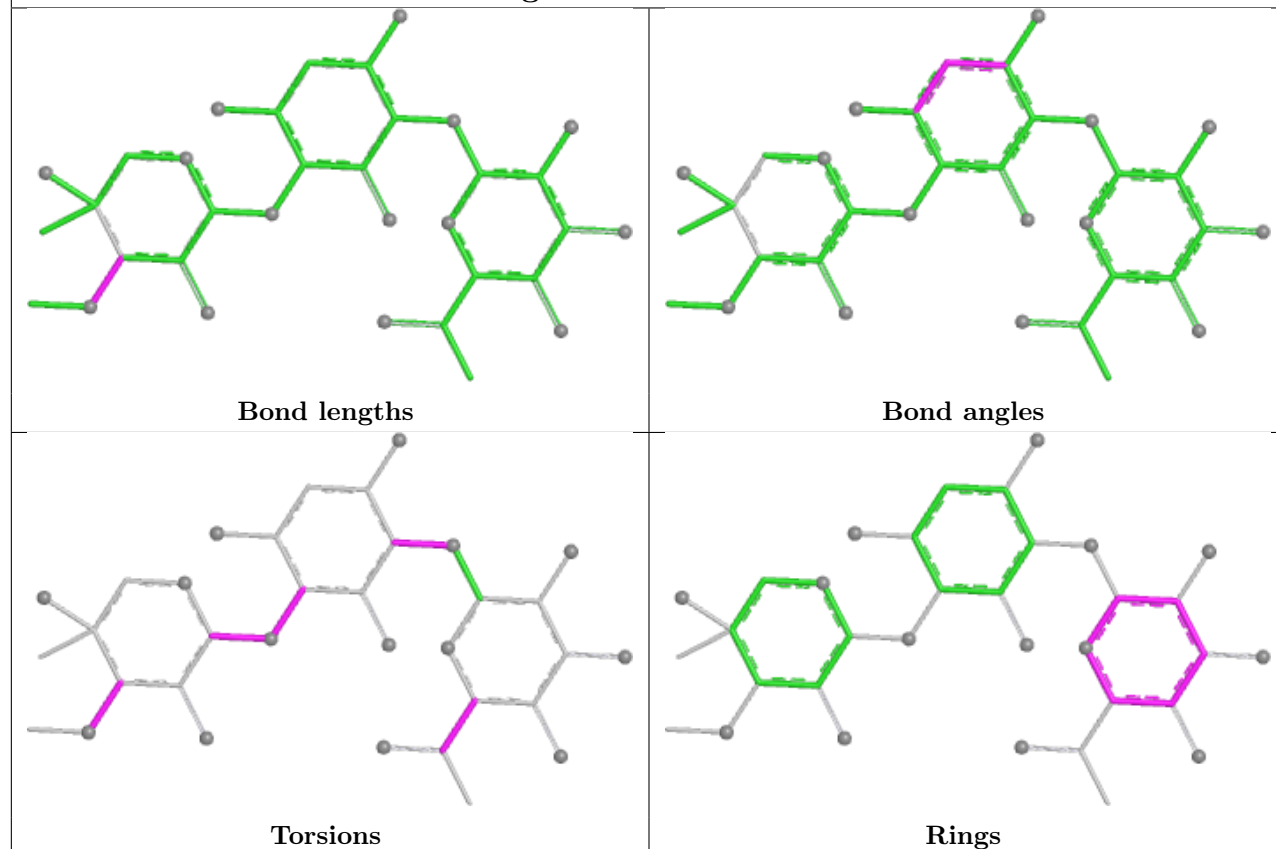
| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 81  | A     | 1802 | GET  | 1       | 0            |
| 81  | 1     | 3408 | GET  | 2       | 0            |
| 81  | 1     | 3413 | GET  | 3       | 0            |
| 81  | 1     | 3403 | GET  | 3       | 0            |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

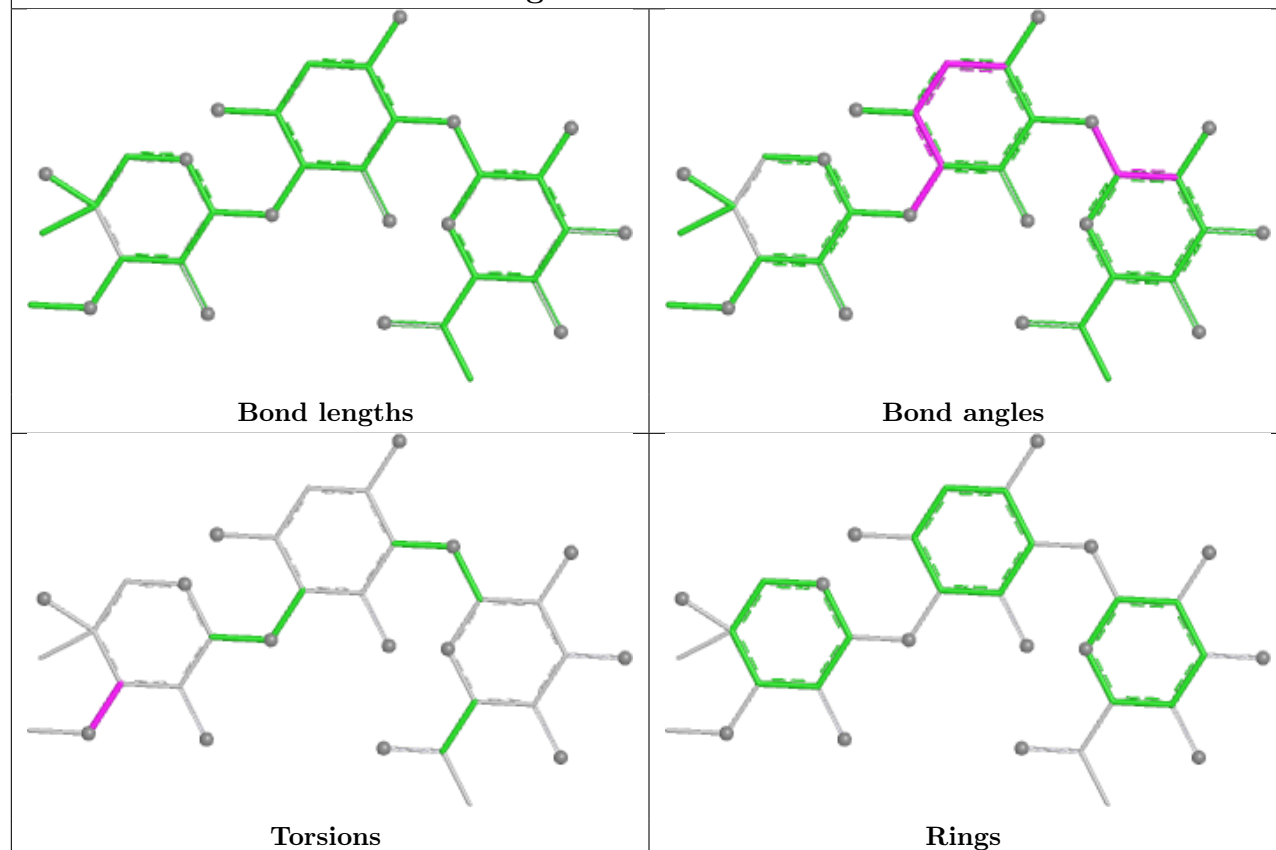


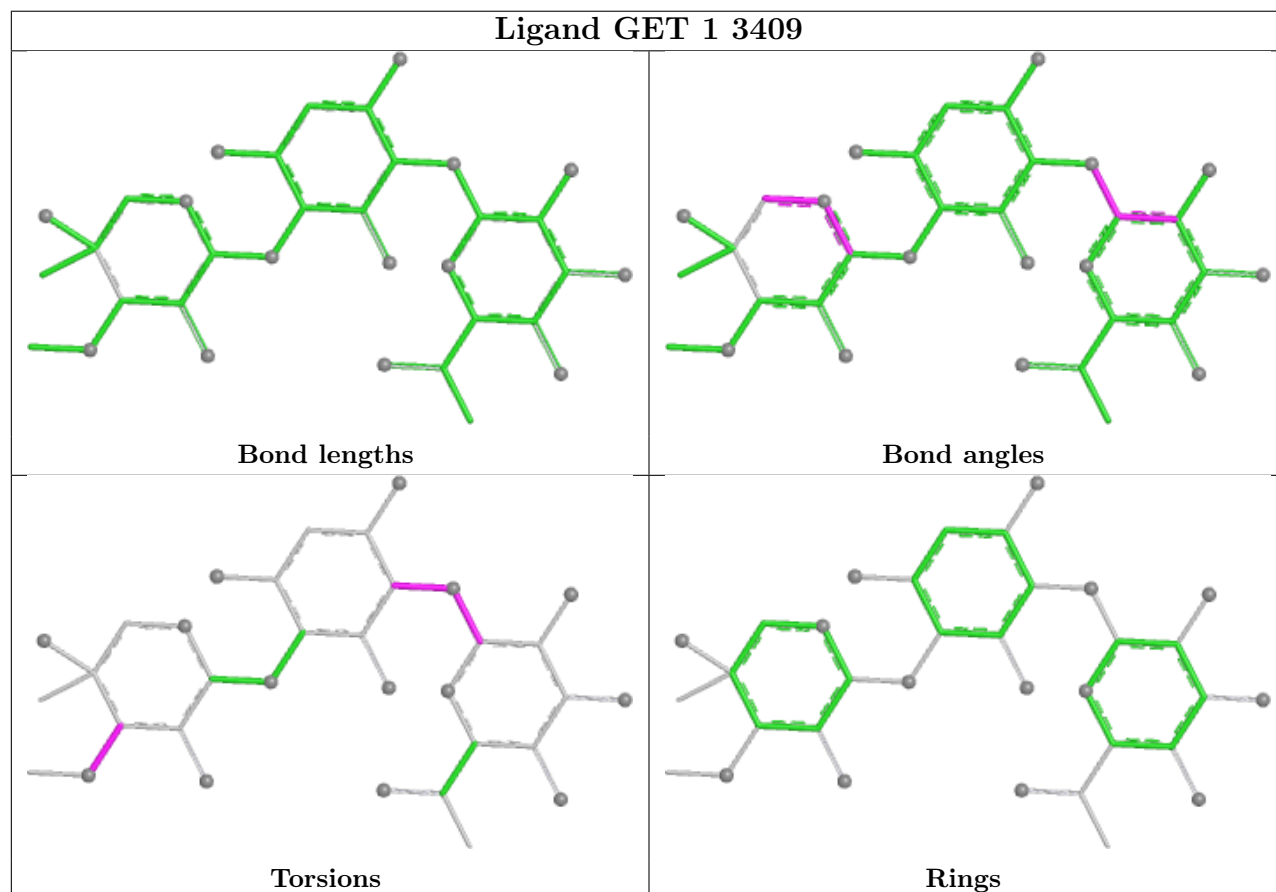
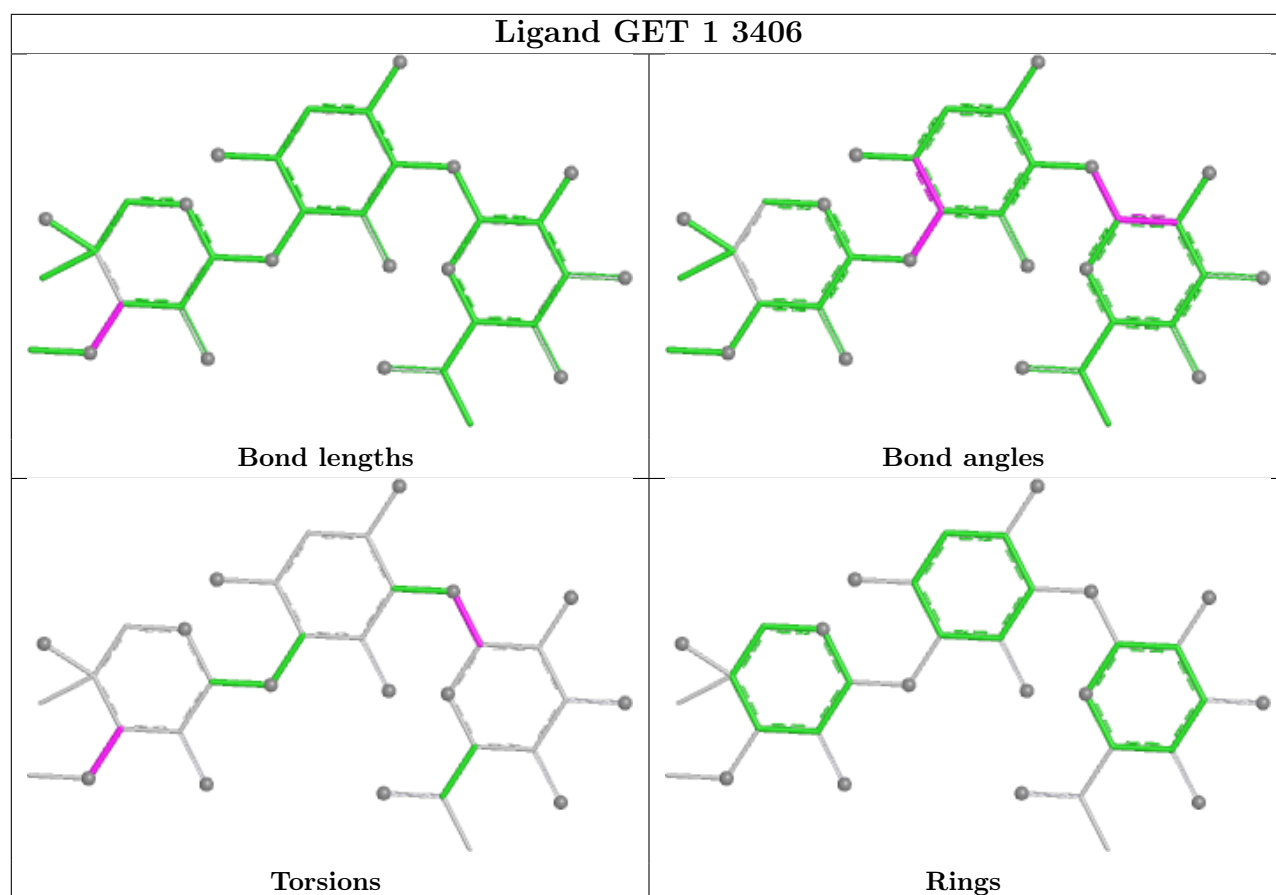


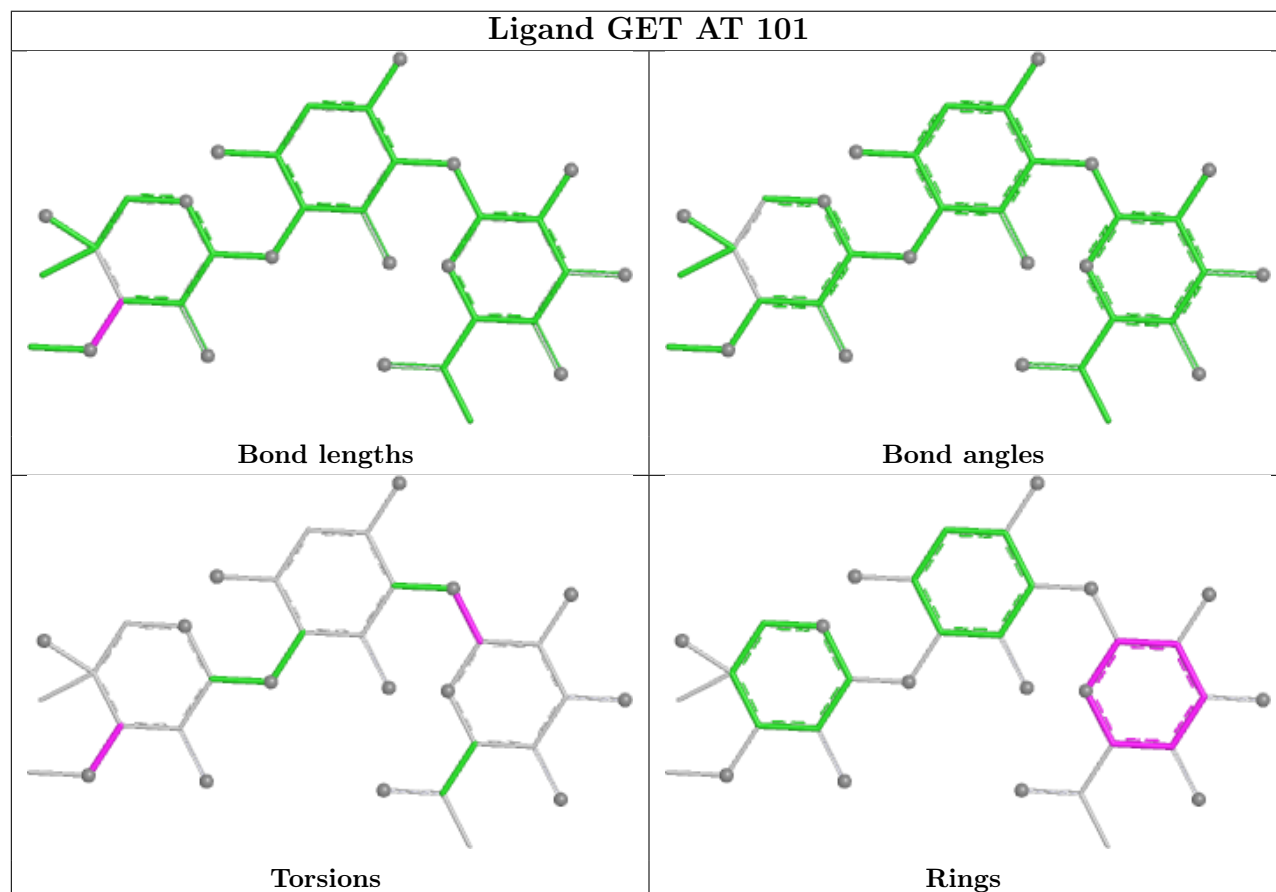
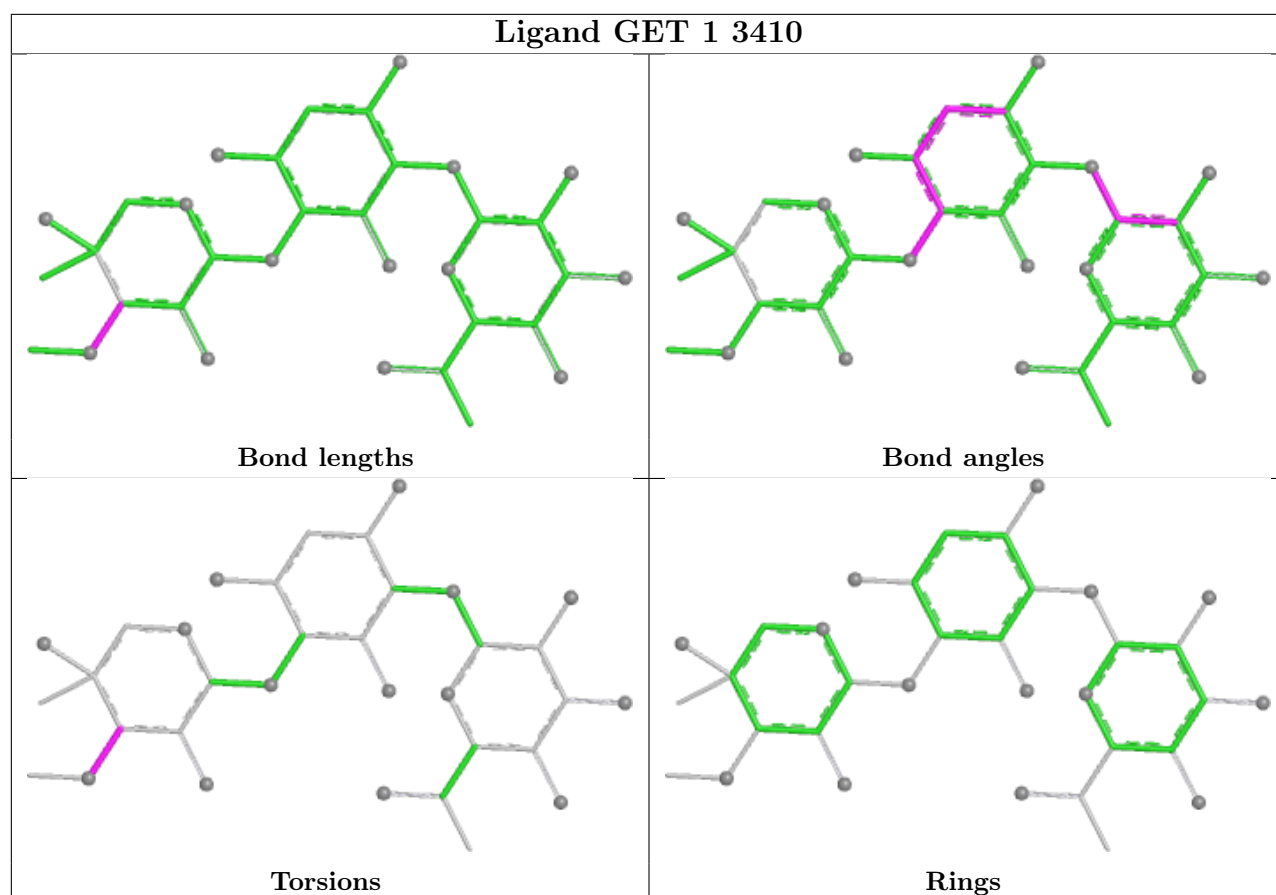
## Ligand GET A 1804

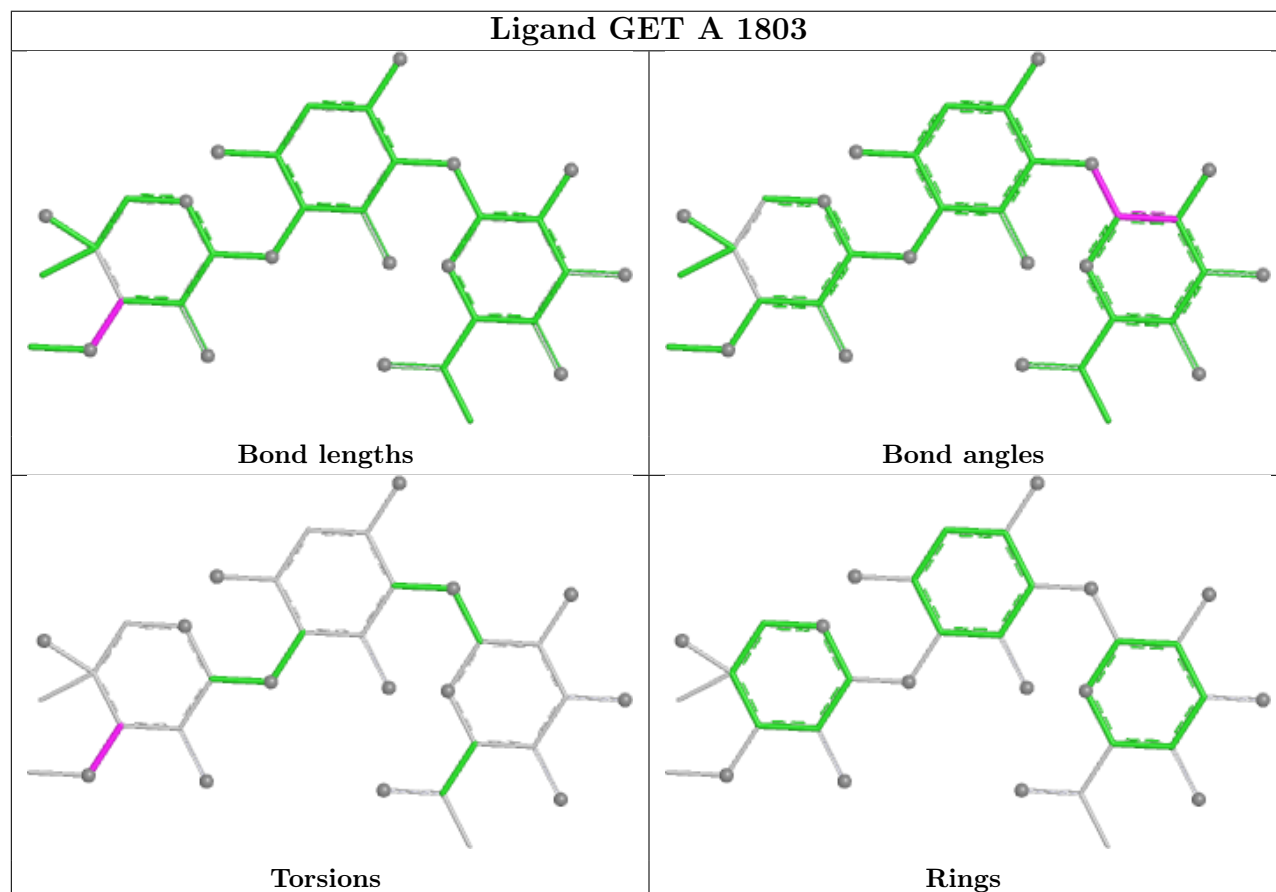
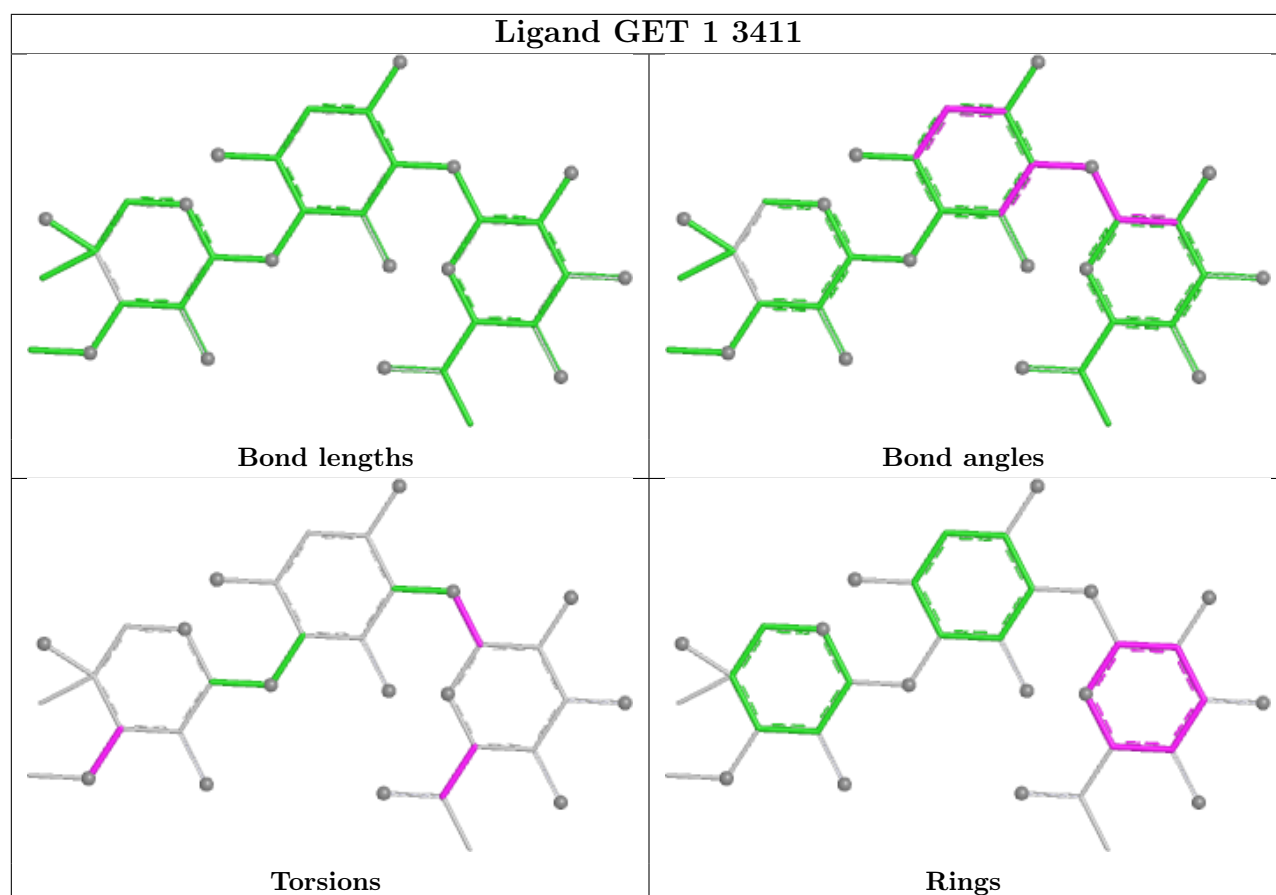


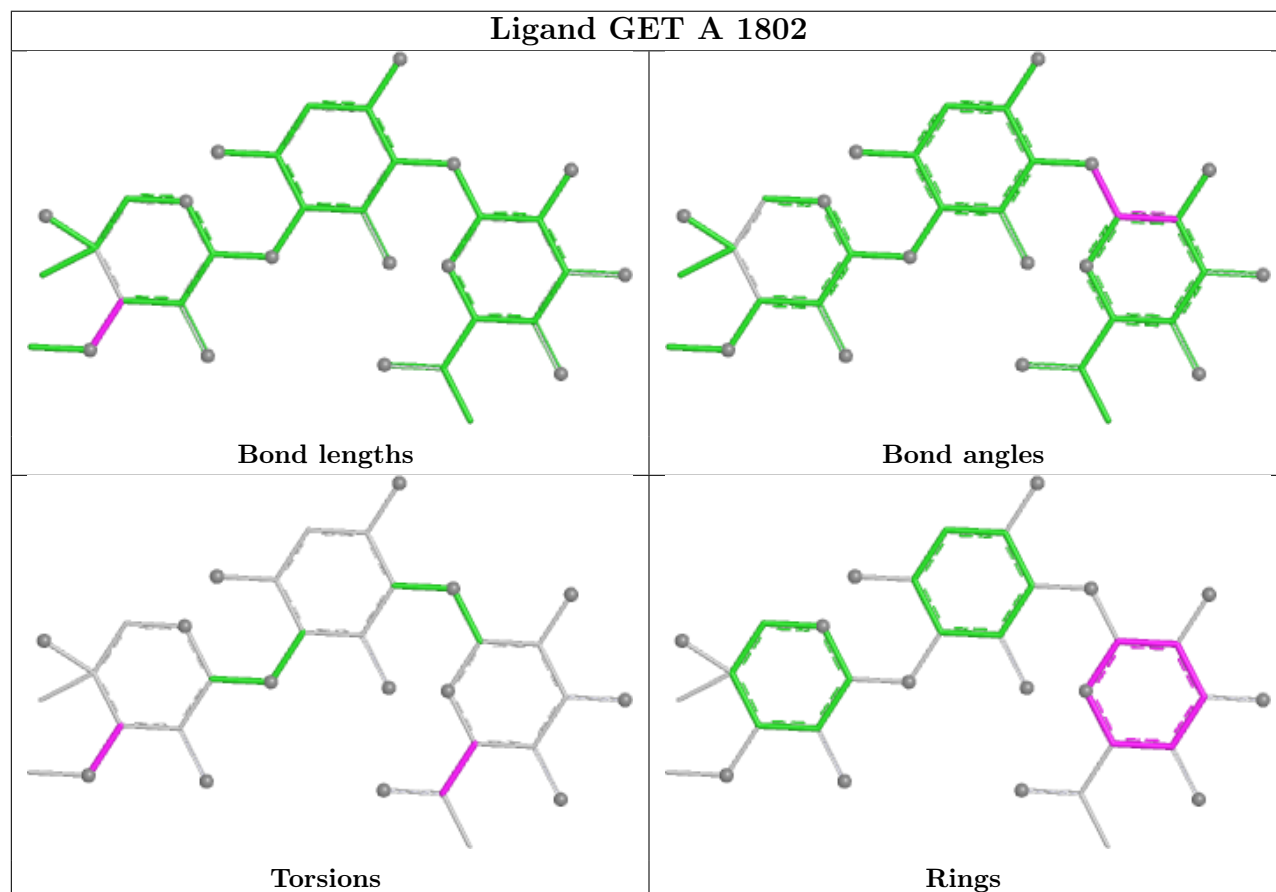
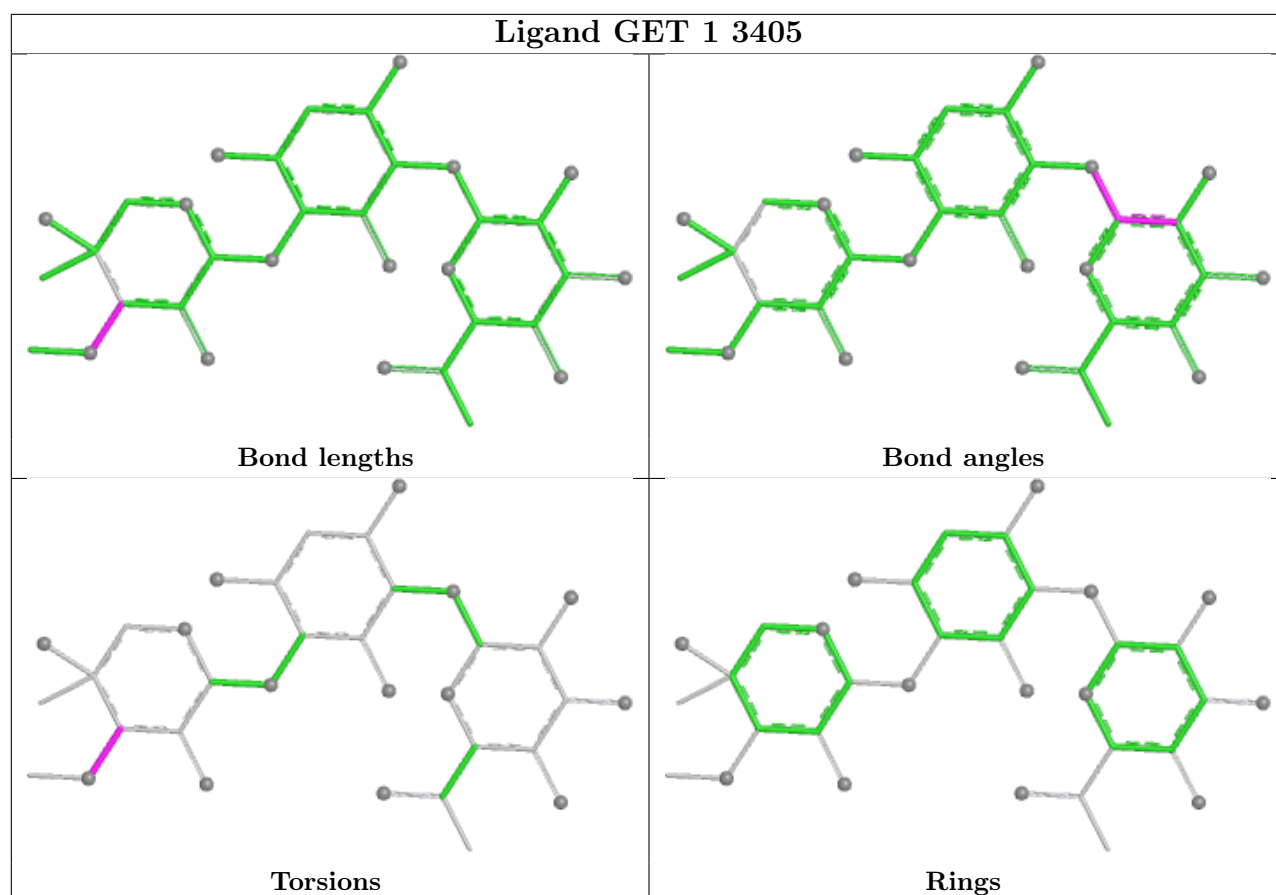
## Ligand GET 1 3407

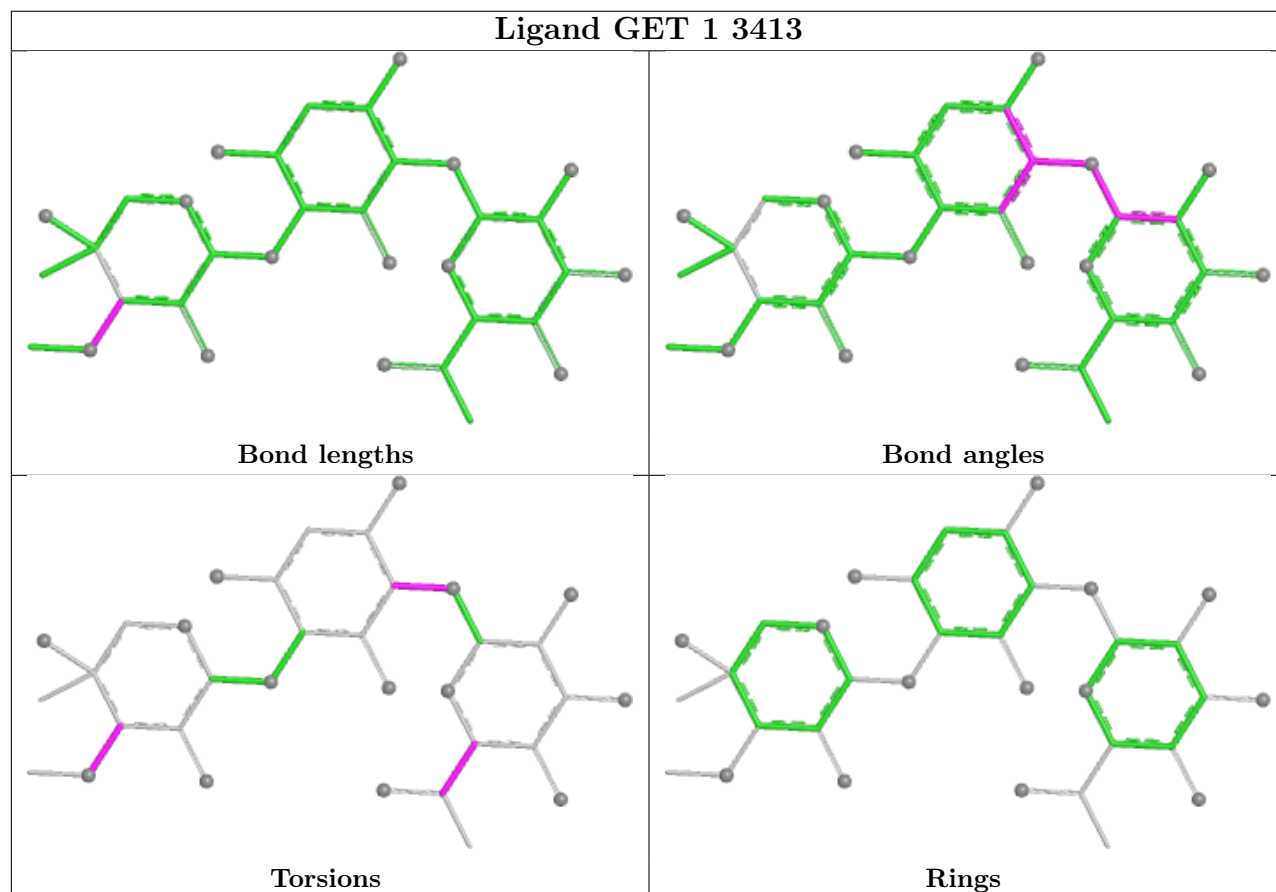
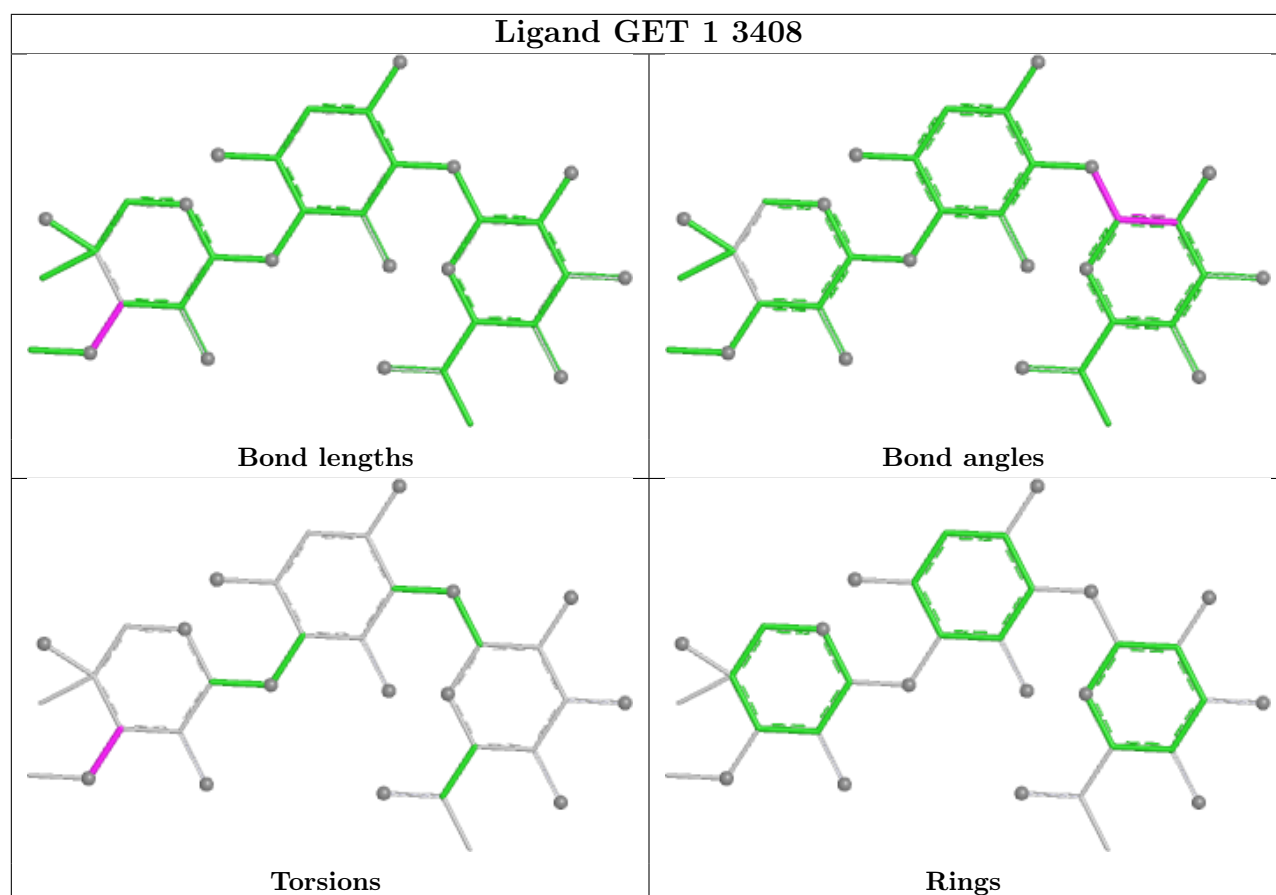


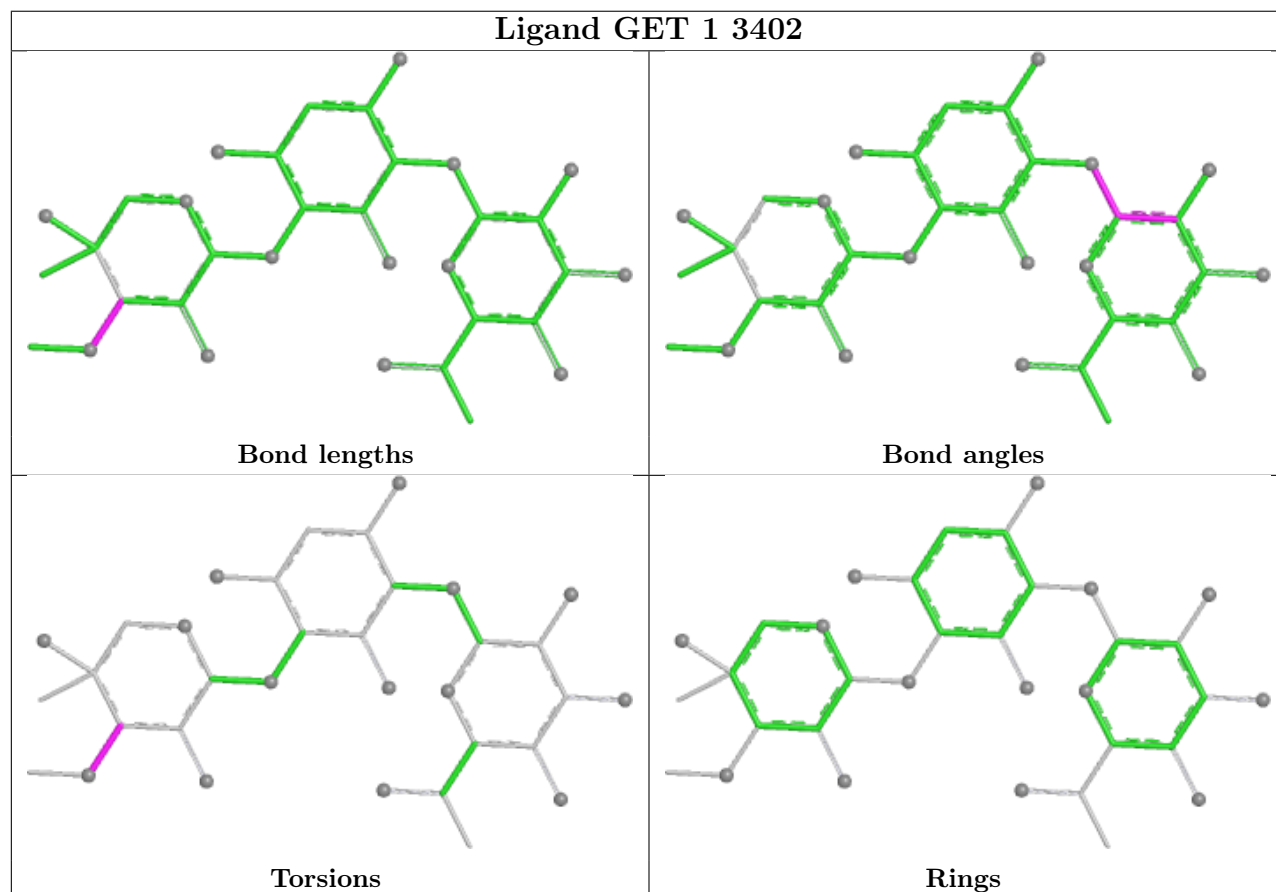
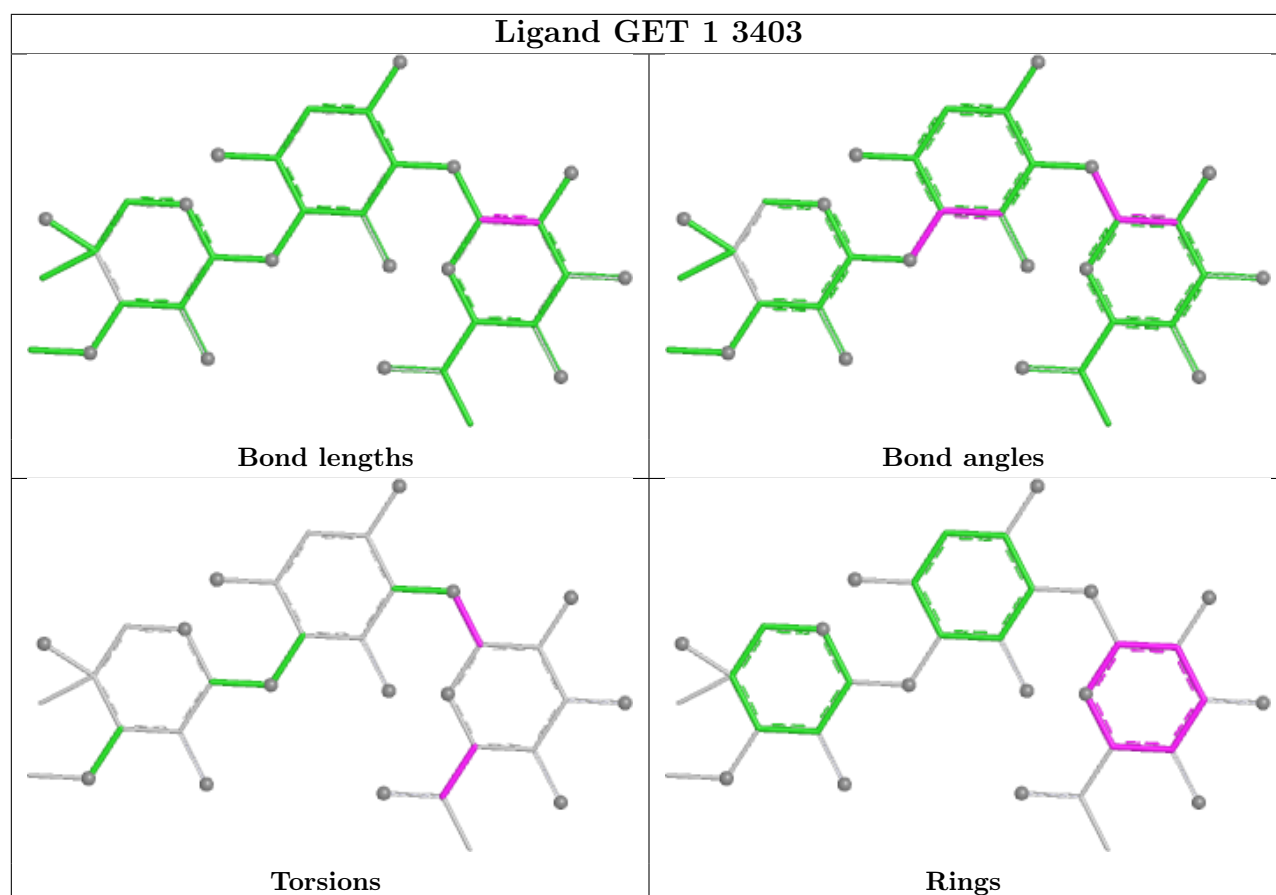












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

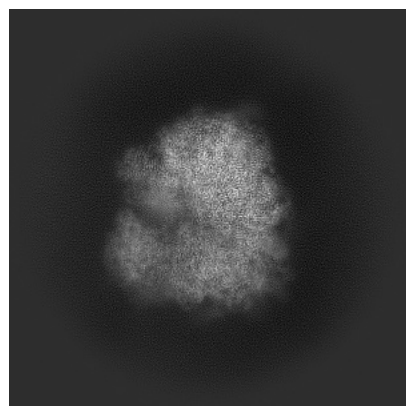
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50990. These allow visual inspection of the internal detail of the map and identification of artifacts.

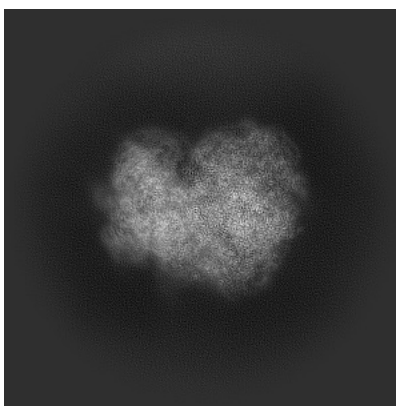
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

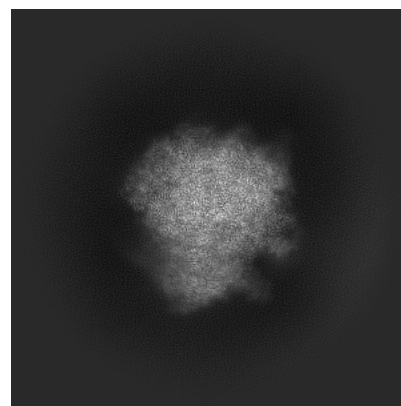
#### 6.1.1 Primary map



X

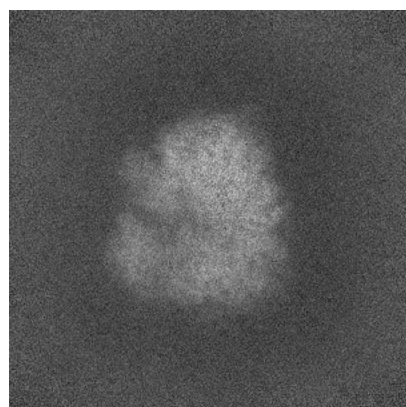


Y

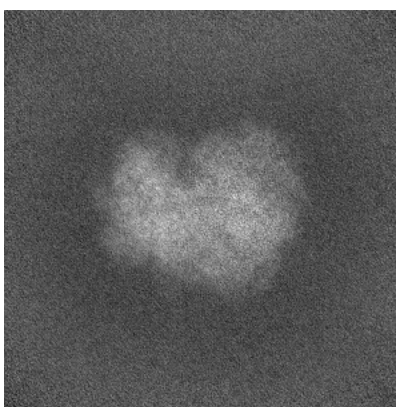


Z

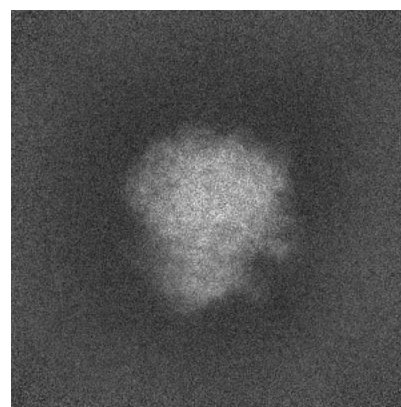
#### 6.1.2 Raw map



X



Y

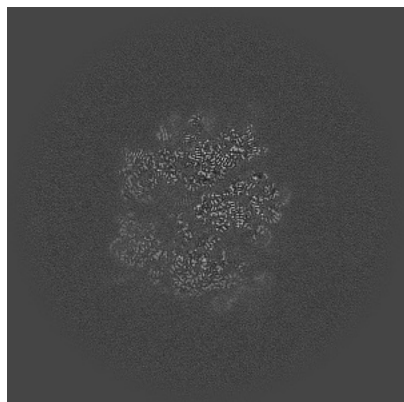


Z

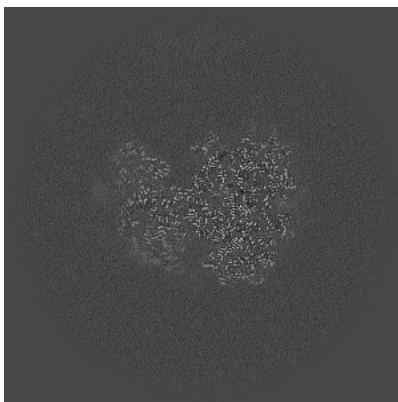
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

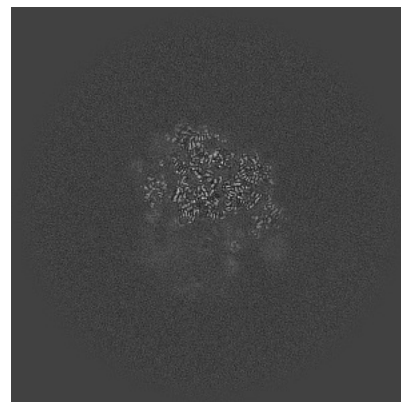
### 6.2.1 Primary map



X Index: 350

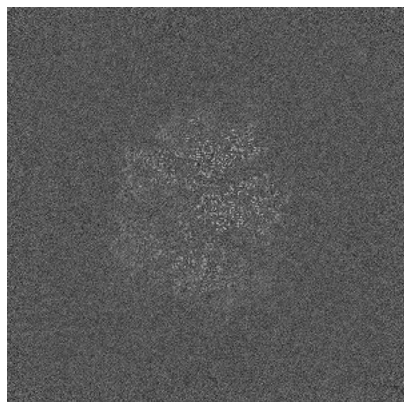


Y Index: 350

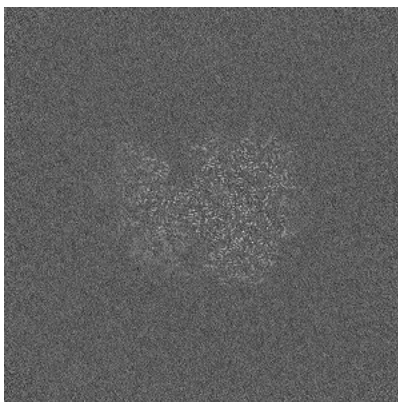


Z Index: 350

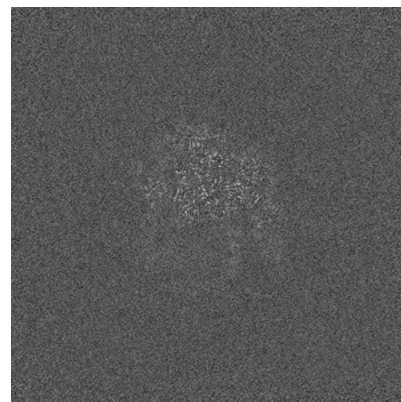
### 6.2.2 Raw map



X Index: 350



Y Index: 350

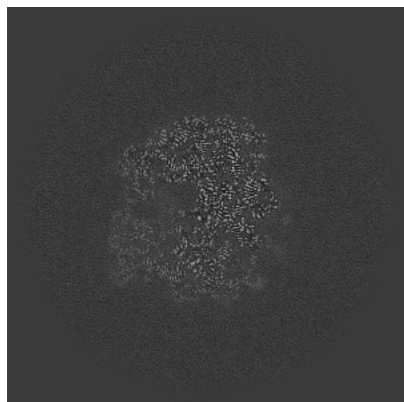


Z Index: 350

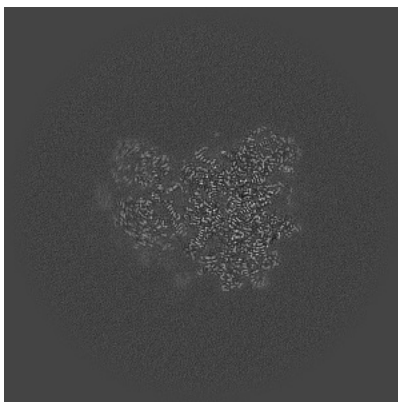
The images above show central slices of the map in three orthogonal directions.

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

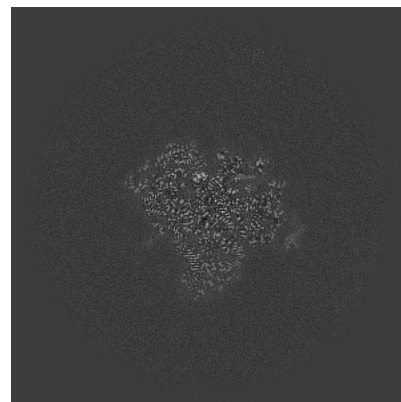
### 6.3.1 Primary map



X Index: 330

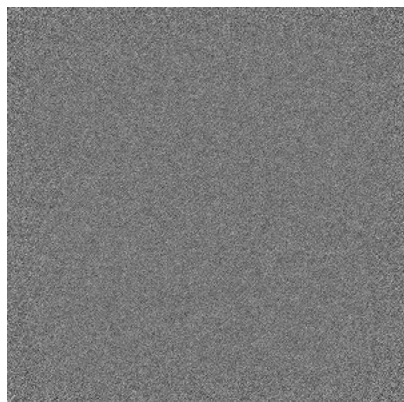


Y Index: 363

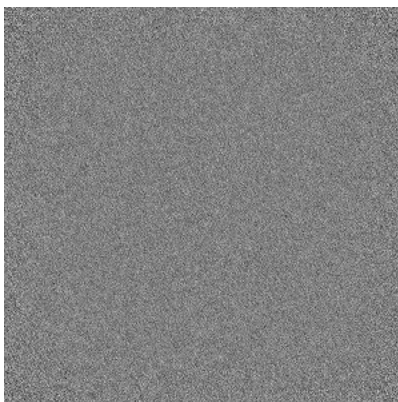


Z Index: 423

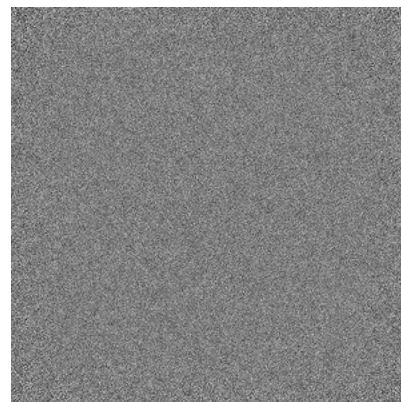
### 6.3.2 Raw map



X Index: 0



Y Index: 0

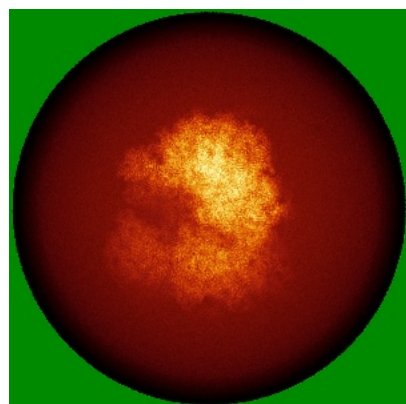


Z Index: 0

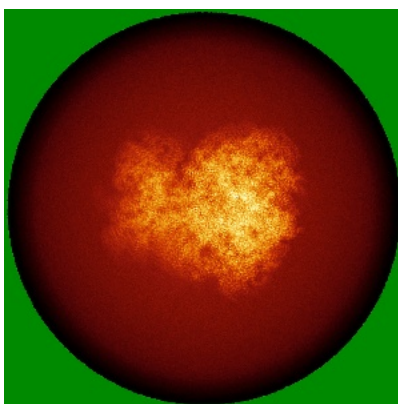
The images above show the largest variance slices of the map in three orthogonal directions.

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

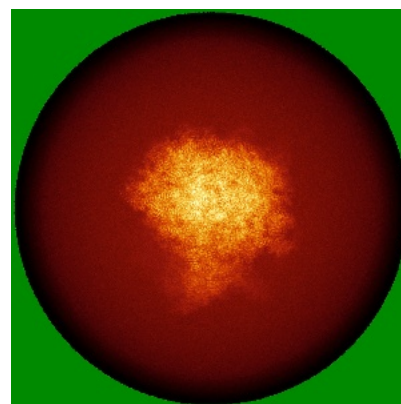
### 6.4.1 Primary map



X

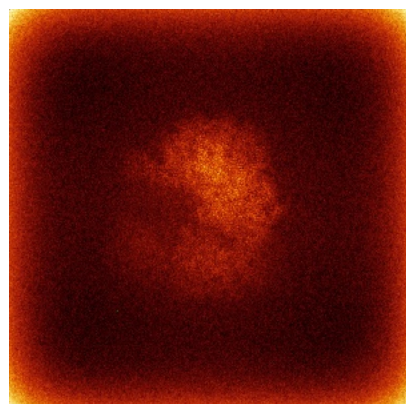


Y

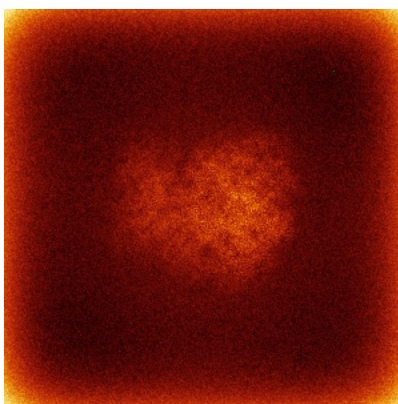


Z

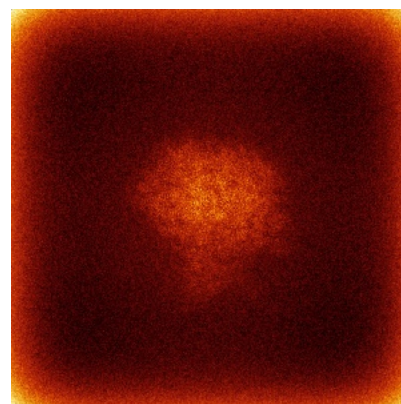
### 6.4.2 Raw map



X



Y

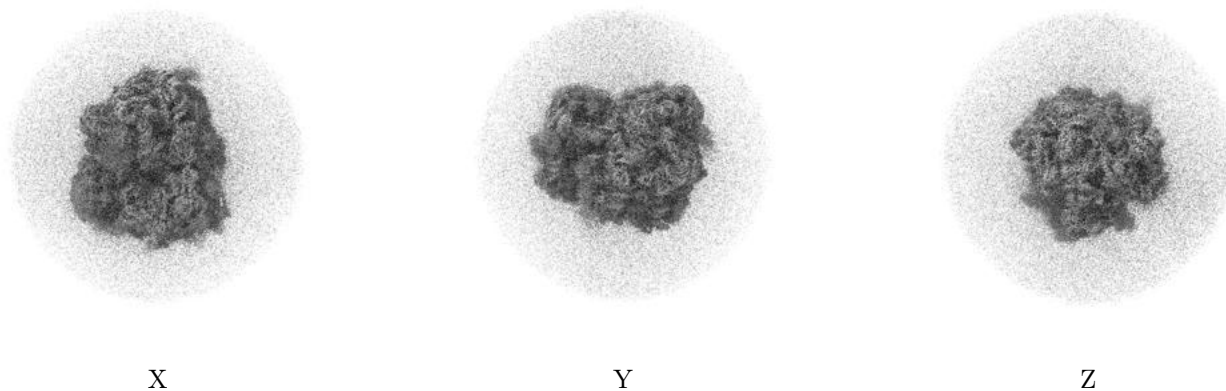


Z

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

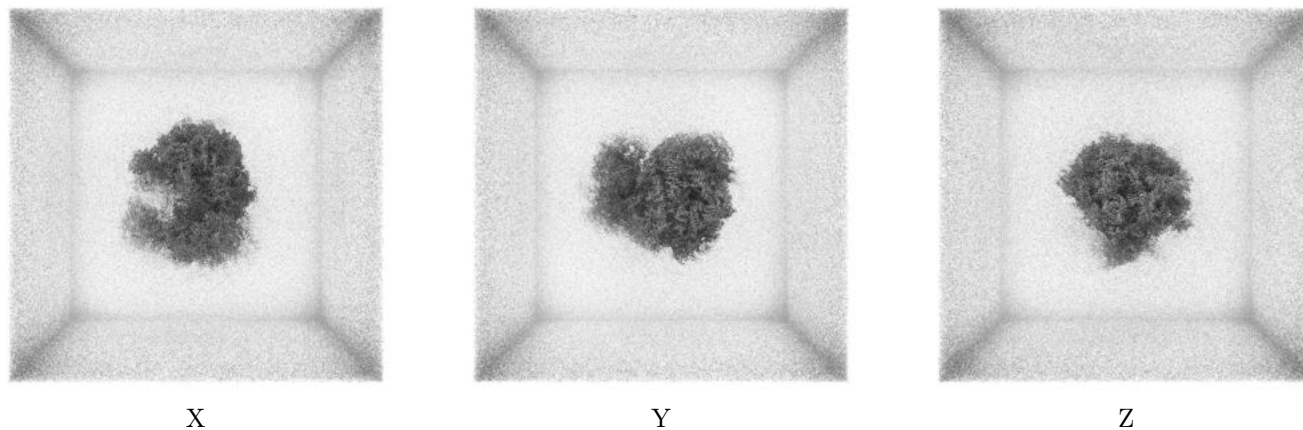
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.168. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

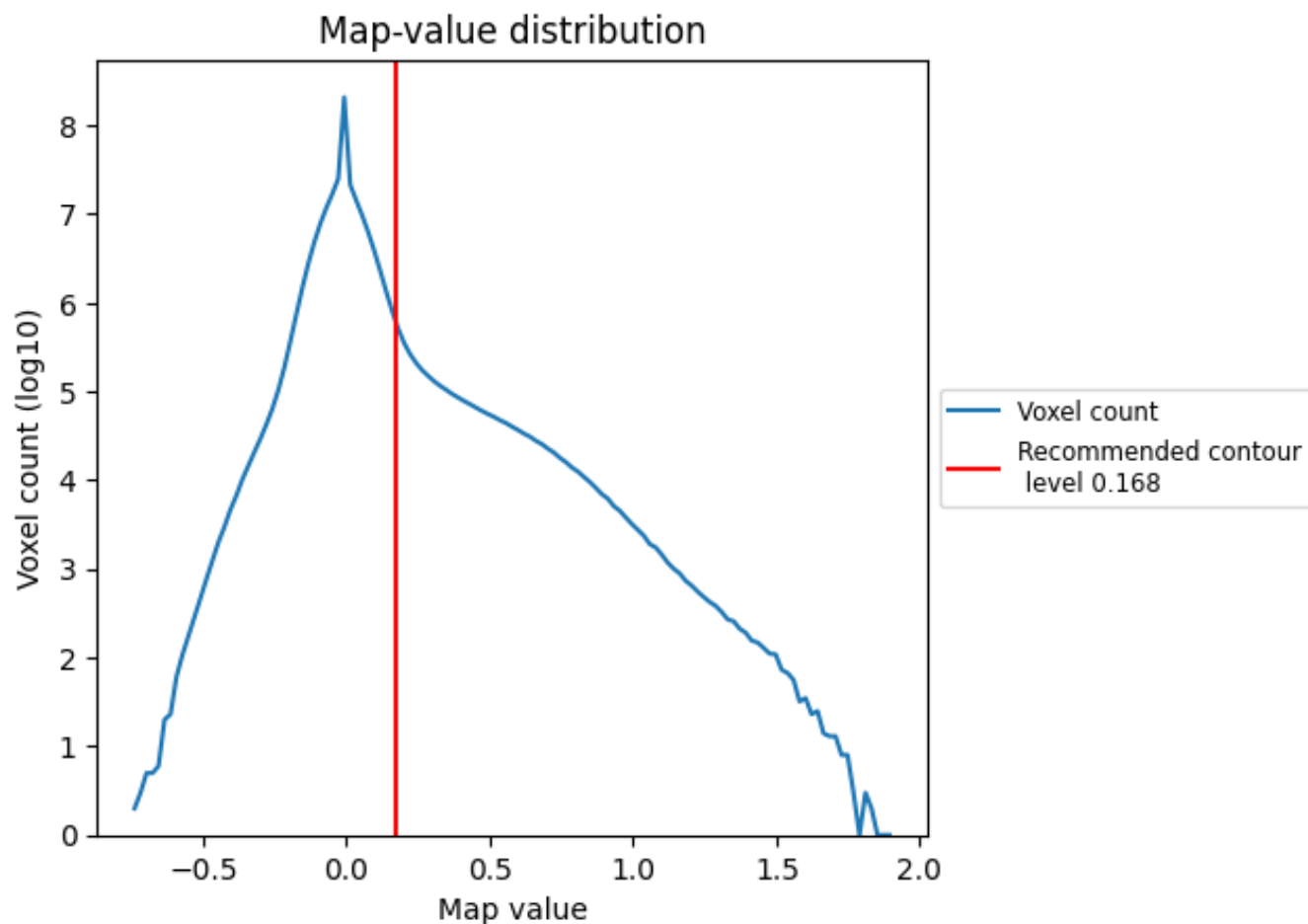
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

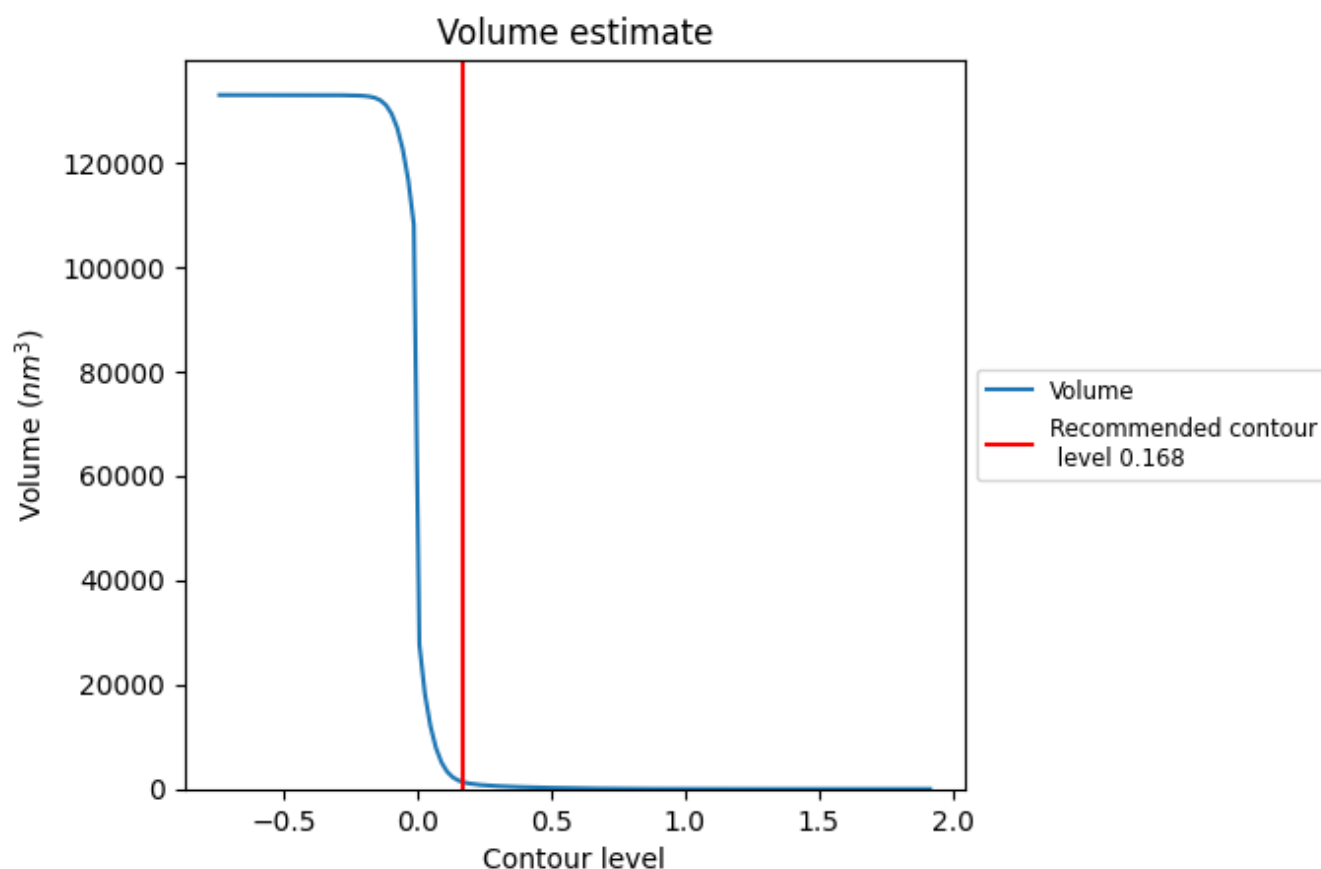
This section contains the results of statistical analysis of the map.

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



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

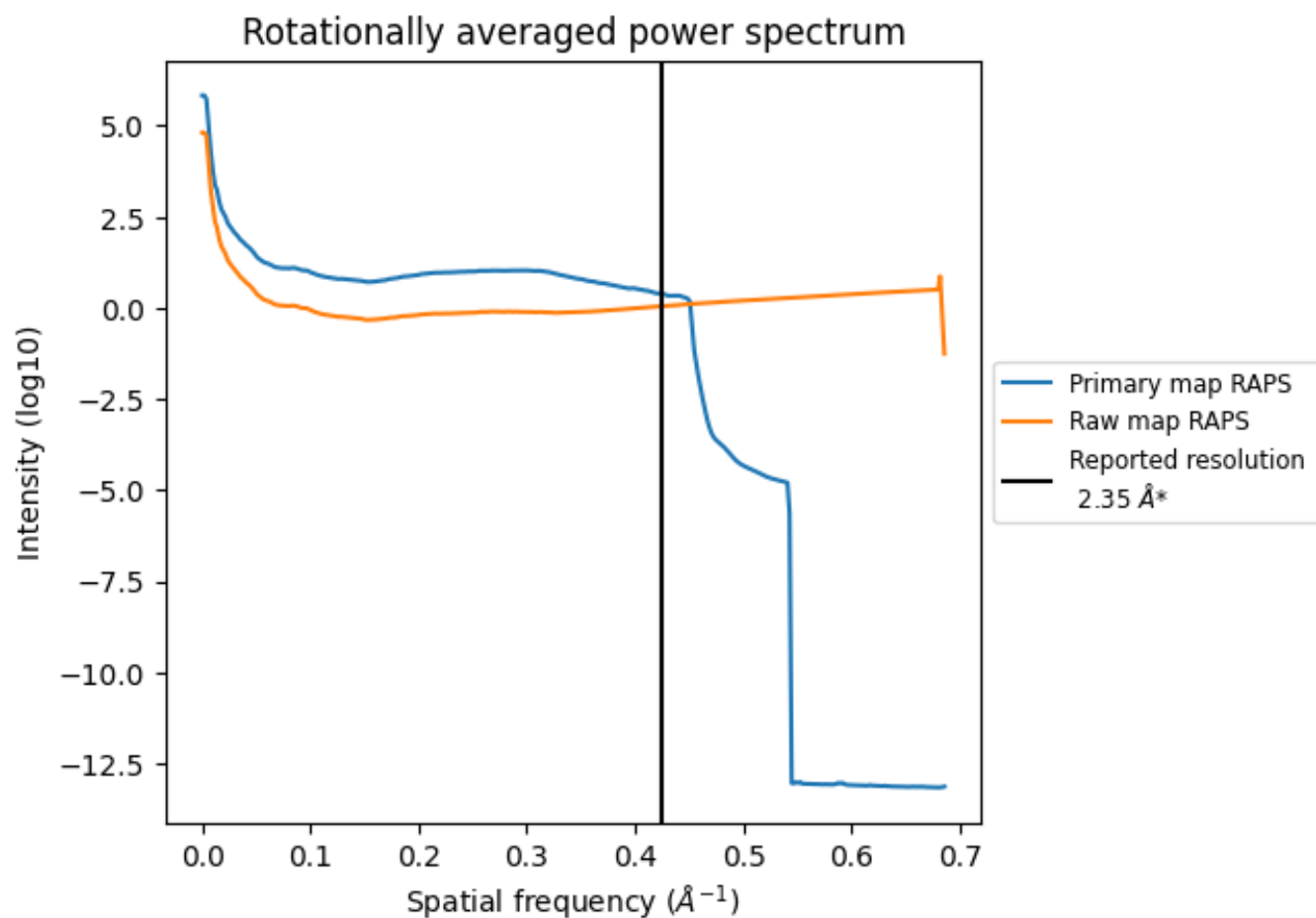
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1357 nm<sup>3</sup>; this corresponds to an approximate mass of 1225 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ

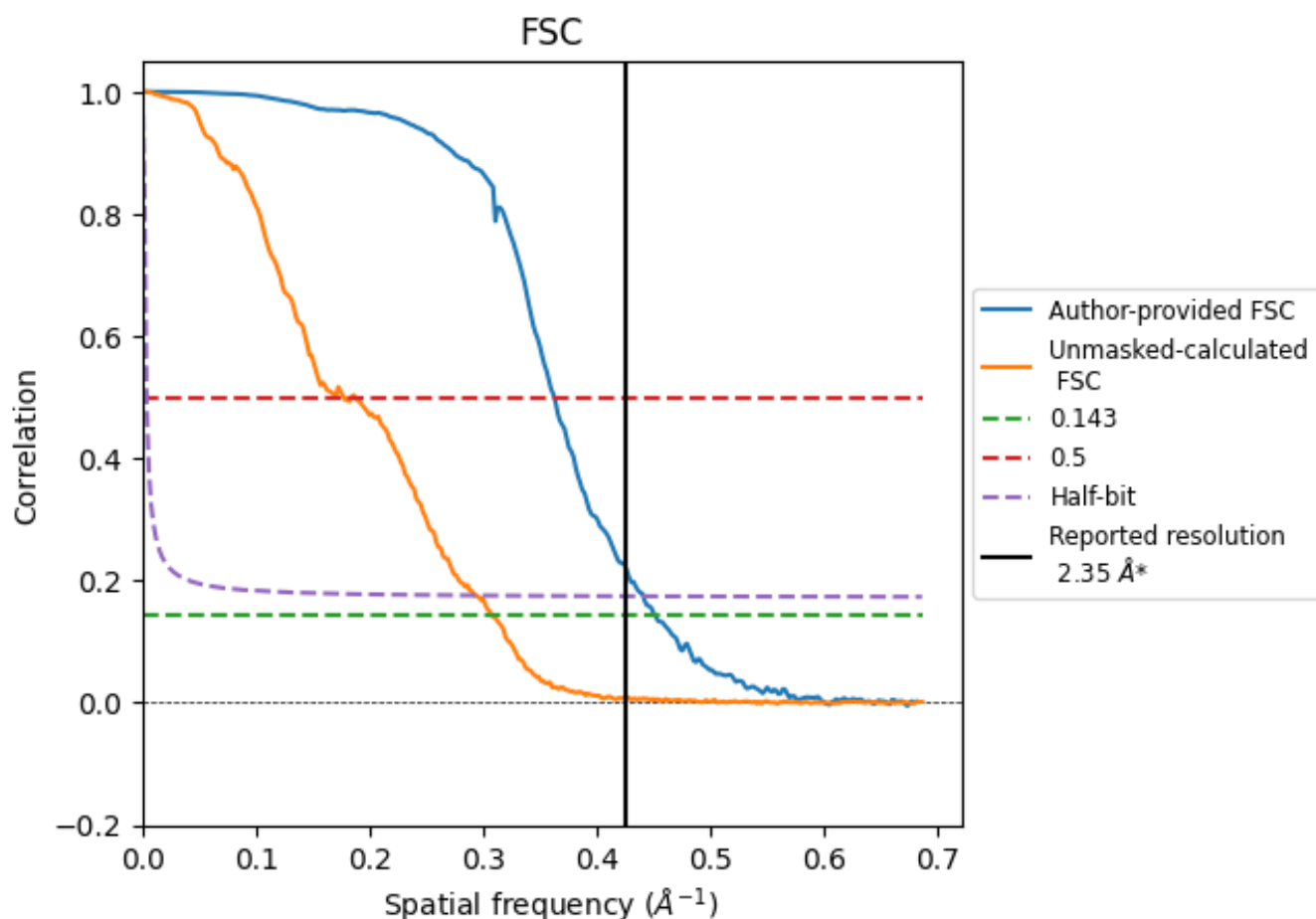


\*Reported resolution corresponds to spatial frequency of 0.426 Å<sup>-1</sup>

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.426  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

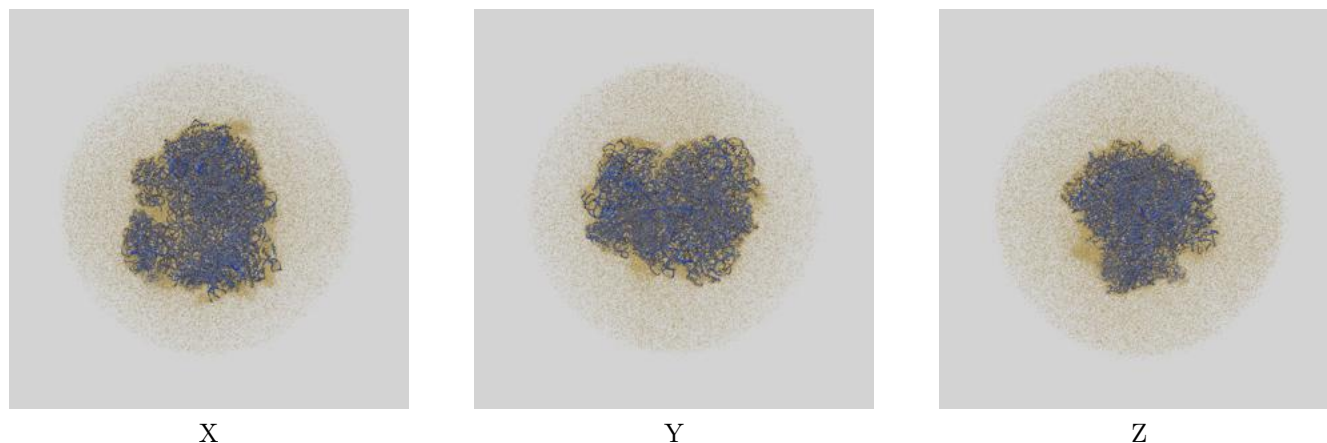
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 2.35                               | -    | -        |
| Author-provided FSC curve | 2.22                               | 2.76 | 2.27     |
| Unmasked-calculated*      | 3.26                               | 5.65 | 3.42     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.26 differs from the reported value 2.35 by more than 10 %

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

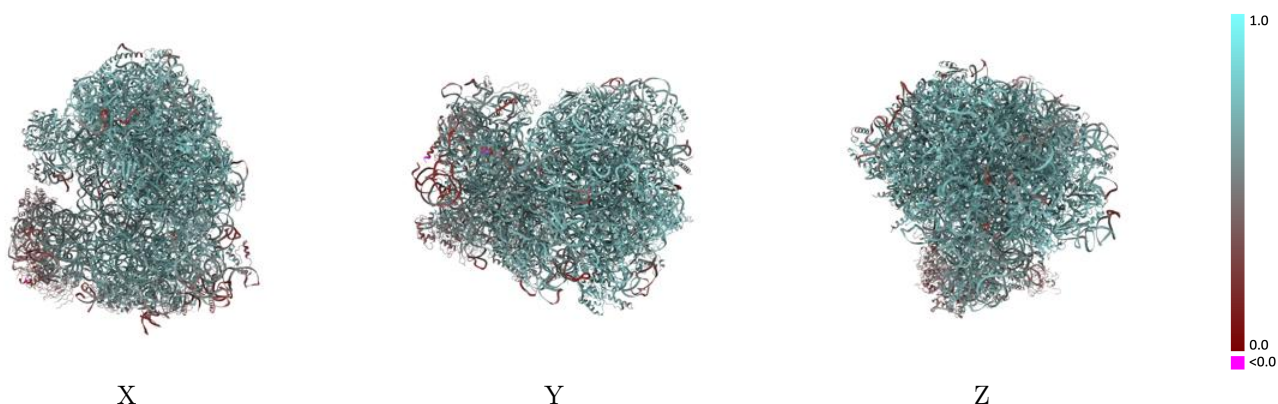
This section contains information regarding the fit between EMDB map EMD-50990 and PDB model 9G30. Per-residue inclusion information can be found in section [3](#) on page [21](#).

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



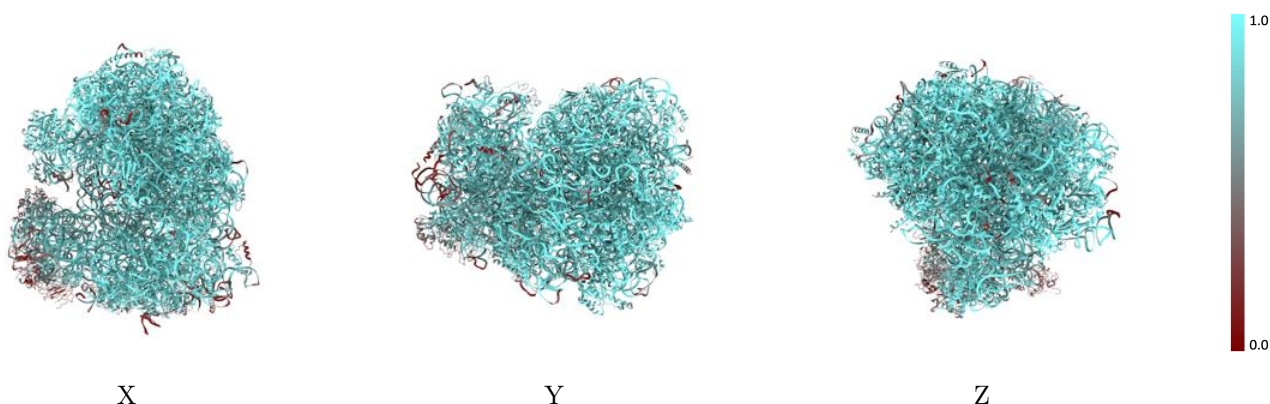
The images above show the 3D surface view of the map at the recommended contour level 0.168 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



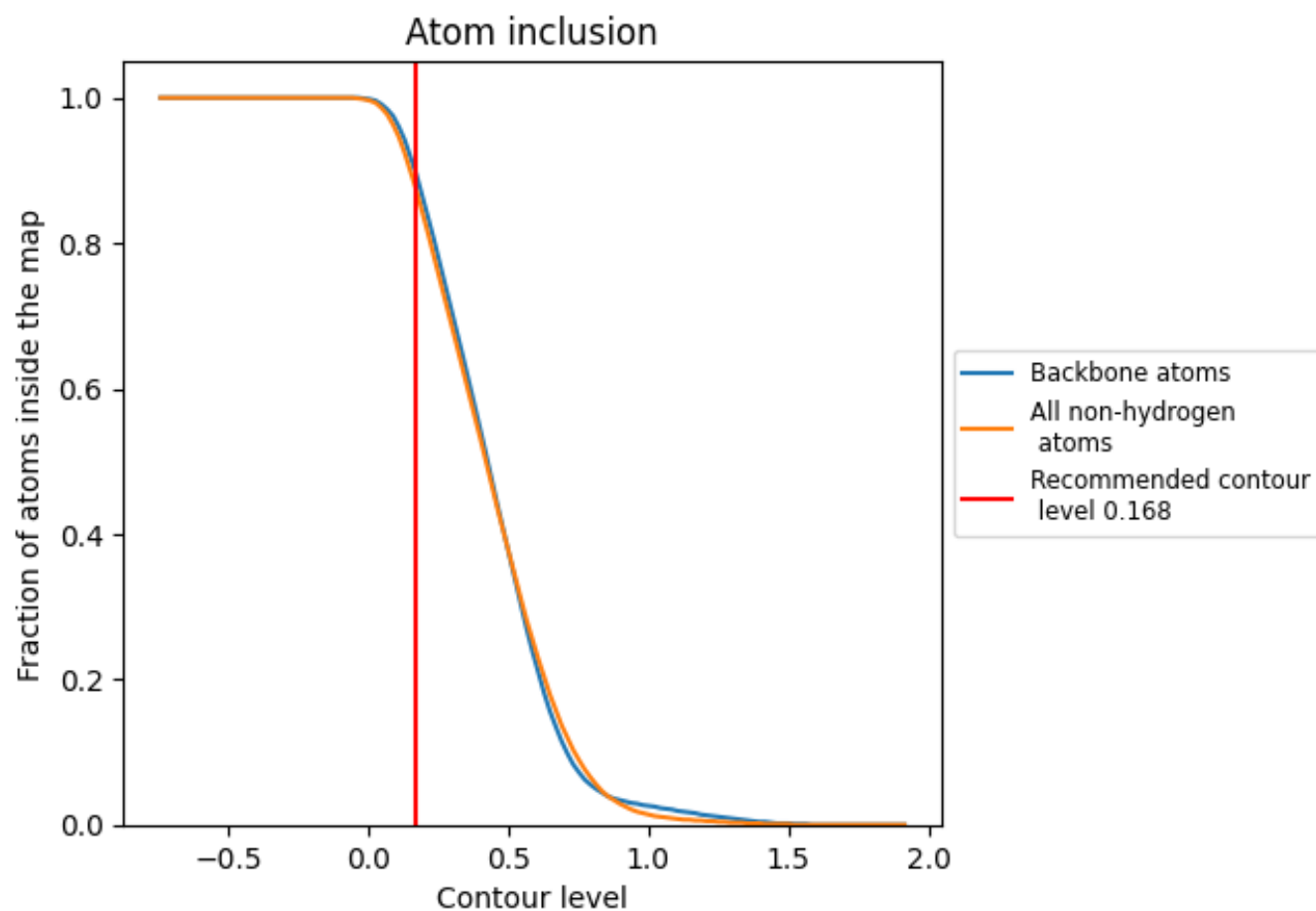
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.168).

## 9.4 Atom inclusion ⓘ



At the recommended contour level, 90% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.168) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.8790   |  0.6160   |
| 0     |  0.9600   |  0.6850   |
| 1     |  0.9570   |  0.6650   |
| 2     |  0.9260   |  0.6640   |
| 3     |  0.9770   |  0.6540   |
| 4     |  0.9740   |  0.6740   |
| 6     |  0.9720   |  0.7010   |
| 7     |  0.9620   |  0.6850   |
| 8     |  0.9570   |  0.6810   |
| 9     |  0.9540   |  0.6790   |
| A     |  0.8710   |  0.5700   |
| AA    |  0.9130   |  0.6470   |
| AB    |  0.9760   |  0.7070   |
| AC    |  0.9290   |  0.6550   |
| AD    |  0.9090  |  0.6490  |
| AE    |  0.9140 |  0.6650 |
| AF    |  0.9640 |  0.6940 |
| AG    |  0.9730 |  0.7010 |
| AH    |  0.9170 |  0.6570 |
| AI    |  0.9330 |  0.6530 |
| AJ    |  0.9050 |  0.6300 |
| AK    |  0.9720 |  0.7060 |
| AL    |  0.8080 |  0.5710 |
| AM    |  0.9690 |  0.6850 |
| AN    |  0.9210 |  0.6640 |
| AO    |  0.7210 |  0.5730 |
| AP    |  0.9030 |  0.6540 |
| AQ    |  0.9200 |  0.6700 |
| AT    |  0.6960 |  0.5050 |
| B     |  0.7420 |  0.5250 |
| C     |  0.6900 |  0.5010 |
| D     |  0.9010 |  0.6200 |
| E     |  0.7080 |  0.5160 |
| F     |  0.8590 |  0.5750 |
| G     |  0.4900 |  0.3920 |



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| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| H     |  0.7640   |  0.5380   |
| I     |  0.6160   |  0.4840   |
| J     |  0.8550   |  0.6120   |
| K     |  0.8170   |  0.5610   |
| L     |  0.5260   |  0.4090   |
| M     |  0.9120   |  0.6440   |
| MR    |  0.8010   |  0.5640   |
| N     |  0.1660   |  0.3040   |
| O     |  0.8790   |  0.6090   |
| P     |  0.7570   |  0.5390   |
| PT    |  0.5960   |  0.5180   |
| Q     |  0.5650   |  0.4570   |
| R     |  0.5670   |  0.4080   |
| S     |  0.5630   |  0.4390   |
| T     |  0.5750   |  0.4290   |
| U     |  0.6230   |  0.4500   |
| V     |  0.6050   |  0.4400   |
| W     |  0.7960  |  0.5530  |
| X     |  0.9310 |  0.6350 |
| Y     |  0.9530 |  0.6720 |
| Z     |  0.7830 |  0.5290 |
| a     |  0.3350 |  0.3540 |
| b     |  0.8330 |  0.5690 |
| c     |  0.7430 |  0.5330 |
| d     |  0.4480 |  0.3740 |
| e     |  0.8970 |  0.6140 |
| f     |  0.7230 |  0.5350 |
| g     |  0.2610 |  0.3350 |
| h     |  0.1540 |  0.3000 |
| j     |  0.9720 |  0.7030 |
| k     |  0.9590 |  0.6940 |
| l     |  0.9400 |  0.6790 |
| m     |  0.8780 |  0.6160 |
| n     |  0.9090 |  0.6310 |
| o     |  0.9410 |  0.6830 |
| p     |  0.9130 |  0.6510 |
| q     |  0.9210 |  0.6500 |
| r     |  0.9210 |  0.6620 |
| s     |  0.7320 |  0.5150 |
| t     |  0.9280 |  0.6620 |
| u     |  0.9410 |  0.6620 |
| v     |  0.9900 |  0.7140 |

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| Chain | Atom inclusion                                                                           | Q-score                                                                                  |
|-------|------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------|
| w     |  0.9550 |  0.6930 |
| x     |  0.9490 |  0.6910 |
| y     |  0.9700 |  0.6960 |
| z     |  0.8940 |  0.6410 |