



## Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 08:14 AM UTC

PDB ID : 9UWH / pdb\_00009uwh  
EMDB ID : EMD-64554  
Title : human mitoribosome trapped by retapamulin  
Authors : Ando, Y.; Nureki, O.; Itoh, Y.  
Deposited on : 2025-05-12  
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

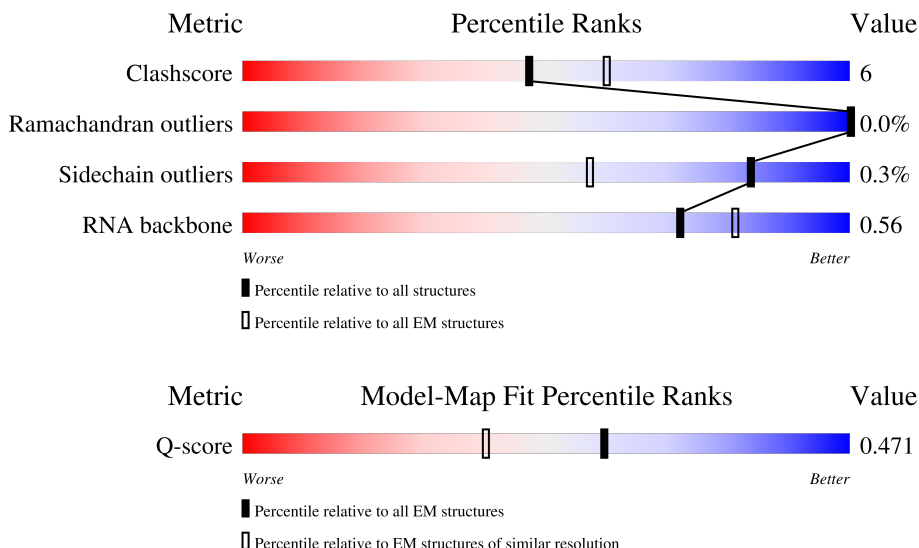
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (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 3.00 Å.

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



| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| RNA backbone          | 8273                        | 3508                        | -                                                        |
| Q-score               | -                           | 25397                       | 14081 ( 2.50 - 3.50 )                                    |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 1561   |                  |
| 2   | B     | 72     |                  |
| 3   | D     | 305    |                  |

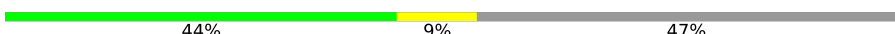
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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 4   | E     | 348    |                  |
| 5   | F     | 311    |                  |
| 6   | H     | 267    |                  |
| 7   | I     | 261    |                  |
| 8   | J     | 192    |                  |
| 9   | K     | 178    |                  |
| 10  | L     | 145    |                  |
| 11  | M     | 296    |                  |
| 12  | N     | 251    |                  |
| 13  | O     | 175    |                  |
| 14  | P     | 180    |                  |
| 15  | Q     | 292    |                  |
| 16  | R     | 149    |                  |
| 17  | S     | 205    |                  |
| 18  | T     | 206    |                  |
| 19  | U     | 153    |                  |
| 20  | V     | 216    |                  |
| 21  | W     | 148    |                  |
| 22  | X     | 256    |                  |
| 23  | Y     | 250    |                  |
| 24  | Z     | 161    |                  |
| 25  | AA    | 954    |                  |
| 26  | AB    | 296    |                  |
| 27  | AC    | 167    |                  |
| 28  | AD    | 430    |                  |

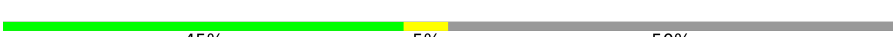
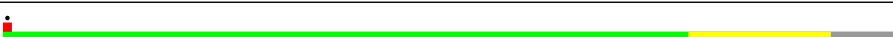
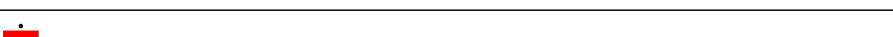
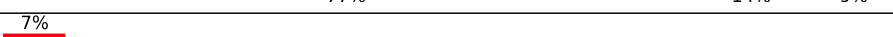
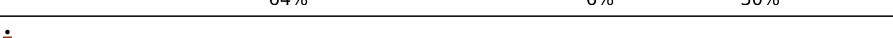
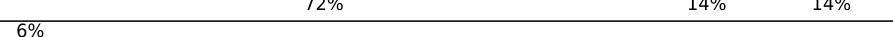
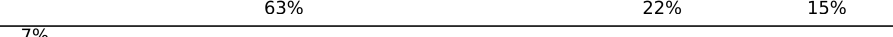
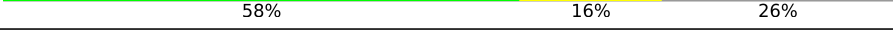
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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 29  | AE    | 125    |    |
| 30  | AF    | 242    |    |
| 31  | AG    | 396    |    |
| 32  | AH    | 201    |    |
| 33  | AI    | 194    |    |
| 34  | AJ    | 138    |    |
| 35  | AK    | 128    |    |
| 36  | AL    | 257    |    |
| 37  | AM    | 137    |    |
| 38  | AN    | 130    |    |
| 39  | AO    | 258    |    |
| 40  | AP    | 142    |   |
| 41  | AQ    | 87     |  |
| 42  | AR    | 360    |  |
| 43  | AS    | 190    |  |
| 44  | AT    | 173    |  |
| 45  | AU    | 205    |  |
| 46  | AV    | 414    |  |
| 47  | AW    | 187    |  |
| 48  | AX    | 398    |  |
| 49  | AY    | 395    |  |
| 50  | AZ    | 106    |  |
| 51  | A0    | 217    |  |
| 52  | A1    | 323    |  |
| 53  | A2    | 118    |  |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 54  | A3    | 199    |    |
| 55  | A4    | 689    |    |
| 56  | Ax    | 71     |    |
| 57  | Az    | 8      |    |
| 58  | 0     | 188    |    |
| 59  | 1     | 65     |    |
| 60  | 2     | 92     |    |
| 61  | 3     | 188    |    |
| 62  | 4     | 103    |    |
| 63  | 5     | 423    |    |
| 64  | 6     | 380    |    |
| 65  | 7     | 338    |    |
| 66  | 8     | 206    |  |
| 67  | 9     | 137    |  |
| 68  | a     | 142    |  |
| 69  | b     | 215    |  |
| 70  | c     | 332    |  |
| 71  | d     | 306    |  |
| 72  | e     | 279    |  |
| 73  | f     | 212    |  |
| 74  | g     | 166    |  |
| 75  | h     | 158    |  |
| 76  | i     | 128    |  |
| 77  | j     | 123    |  |
| 78  | k     | 112    |  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 79  | l     | 138    |                  |
| 80  | m     | 128    |                  |
| 81  | o     | 102    |                  |
| 82  | p     | 206    |                  |
| 83  | q     | 222    |                  |
| 84  | r     | 196    |                  |
| 85  | s     | 439    |                  |
| 86  | t     | 198    |                  |

## 2 Entry composition

There are 96 unique types of molecules in this entry. The entry contains 171472 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S mitochondrial rRNA.

| Mol | Chain | Residues | Atoms |       |      |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|-------|
| 1   | A     | 1523     | Total | C     | N    | O     | P    | 0       | 0     |
|     |       |          | 32331 | 14510 | 5827 | 10471 | 1523 |         |       |

- Molecule 2 is a RNA chain called mitochondrial tRNAVal.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 2   | B     | 72       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1524  | 685 | 269 | 498 | 72 |         |       |

- Molecule 3 is a protein called Large ribosomal subunit protein uL2m.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 3   | D     | 238      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1859  | 1157 | 376 | 317 | 9 |         |       |

- Molecule 4 is a protein called Large ribosomal subunit protein uL3m.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 4   | E     | 305      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2406  | 1545 | 418 | 432 | 11 |         |       |

- Molecule 5 is a protein called Large ribosomal subunit protein uL4m.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 5   | F     | 252      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2031  | 1305 | 370 | 350 | 6 |         |       |

- Molecule 6 is a protein called Large ribosomal subunit protein bL9m.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 6   | H     | 100      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 823   | 522 | 159 | 142 |         |       |

- Molecule 7 is a protein called Large ribosomal subunit protein uL10m.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 7   | I     | 169      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1362  | 877 | 247 | 228 | 10 |         |       |

- Molecule 8 is a protein called Large ribosomal subunit protein uL11m.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 8   | J     | 175      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1330  | 847 | 237 | 244 | 2 |         |       |

- Molecule 9 is a protein called Large ribosomal subunit protein uL13m.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 9   | K     | 178      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1455  | 936 | 259 | 253 | 7 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment     | Reference  |
|-------|---------|----------|--------|-------------|------------|
| K     | 1       | ACE      | -      | acetylation | UNP Q9BYD1 |

- Molecule 10 is a protein called Large ribosomal subunit protein uL14m.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 10  | L     | 115      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 890   | 559 | 171 | 155 | 5 |         |       |

- Molecule 11 is a protein called Large ribosomal subunit protein uL15m.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 11  | M     | 289      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2314  | 1476 | 427 | 405 | 6 |         |       |

- Molecule 12 is a protein called Large ribosomal subunit protein uL16m.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 12  | N     | 222      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1786  | 1143 | 326 | 307 | 10 |         |       |

- Molecule 13 is a protein called Large ribosomal subunit protein bL17m.



| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 13  | O     | 154      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1259  | 792 | 241 | 219 | 7 |         |       |

- Molecule 14 is a protein called Large ribosomal subunit protein uL18m.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 14  | P     | 144      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1173  | 733 | 224 | 211 | 5 |         |       |

- Molecule 15 is a protein called Large ribosomal subunit protein bL19m.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 15  | Q     | 239      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1990  | 1277 | 353 | 351 | 9 |         |       |

- Molecule 16 is a protein called Large ribosomal subunit protein bL20m.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 16  | R     | 140      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1154  | 732 | 231 | 187 | 4 |         |       |

- Molecule 17 is a protein called Large ribosomal subunit protein bL21m.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 17  | S     | 161      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1293  | 835 | 227 | 227 | 4 |         |       |

- Molecule 18 is a protein called Large ribosomal subunit protein uL22m.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 18  | T     | 166      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1369  | 875 | 254 | 233 | 7 |         |       |

- Molecule 19 is a protein called Large ribosomal subunit protein uL23m.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19  | U     | 153      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1251  | 788 | 234 | 226 | 3 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment     | Reference  |
|-------|---------|----------|--------|-------------|------------|
| U     | 1       | ACE      | -      | acetylation | UNP Q16540 |

- Molecule 20 is a protein called Large ribosomal subunit protein uL24m.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 20  | V     | 205      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1676  | 1068 | 298 | 302 | 8 |         |       |

- Molecule 21 is a protein called Large ribosomal subunit protein bL27m.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 21  | W     | 116      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 904   | 577 | 171 | 153 | 3 |         |       |

- Molecule 22 is a protein called Large ribosomal subunit protein bL28m.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 22  | X     | 244      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2044  | 1322 | 352 | 365 | 5 |         |       |

- Molecule 23 is a protein called Large ribosomal subunit protein uL29m.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 23  | Y     | 181      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1556  | 995 | 298 | 259 | 4 |         |       |

- Molecule 24 is a protein called Large ribosomal subunit protein uL30m.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 24  | Z     | 122      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 996   | 636 | 186 | 171 | 3 |         |       |

- Molecule 25 is a RNA chain called 12S mitochondrial rRNA.

| Mol | Chain | Residues | Atoms |      |      |      |     | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|-----|---------|-------|
| 25  | AA    | 954      | Total | C    | N    | O    | P   | 0       | 0     |
|     |       |          | 20260 | 9088 | 3647 | 6571 | 954 |         |       |

- Molecule 26 is a protein called Small ribosomal subunit protein uS2m.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 26  | AB    | 225      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1828  | 1164 | 331 | 323 | 10 |         |       |

- Molecule 27 is a protein called Small ribosomal subunit protein uS3m.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 27  | AC    | 132      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1083  | 699 | 195 | 185 | 4 |         |       |

- Molecule 28 is a protein called Small ribosomal subunit protein uS5m.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 28  | AD    | 343      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2731  | 1713 | 518 | 487 | 13 |         |       |

- Molecule 29 is a protein called Small ribosomal subunit protein bS6m.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 29  | AE    | 122      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 972   | 614 | 177 | 177 | 4 |         |       |

- Molecule 30 is a protein called Small ribosomal subunit protein uS7m.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 30  | AF    | 208      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1725  | 1104 | 312 | 298 | 11 |         |       |

- Molecule 31 is a protein called Small ribosomal subunit protein uS9m.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 31  | AG    | 311      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2561  | 1627 | 454 | 466 | 14 |         |       |

- Molecule 32 is a protein called Small ribosomal subunit protein uS10m.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 32  | AH    | 140      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1152  | 745 | 194 | 210 | 3 |         |       |

- Molecule 33 is a protein called Small ribosomal subunit protein uS11m.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 33  | AI    | 137      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1020  | 642 | 192 | 182 | 4 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| AI    | 184     | 5F0      | ASN    | conflict | UNP P82912 |

- Molecule 34 is a protein called Small ribosomal subunit protein uS12m.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 34  | AJ    | 108      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 839   | 521 | 169 | 143 | 6 |         |       |

- Molecule 35 is a protein called Small ribosomal subunit protein uS14m.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 35  | AK    | 101      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 862   | 537 | 179 | 141 | 5 |         |       |

- Molecule 36 is a protein called Small ribosomal subunit protein uS15m.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 36  | AL    | 174      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1453  | 925 | 270 | 251 | 7 |         |       |

- Molecule 37 is a protein called Small ribosomal subunit protein bS16m.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 37  | AM    | 119      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 942   | 594 | 185 | 157 | 6 |         |       |

- Molecule 38 is a protein called Small ribosomal subunit protein uS17m.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 38  | AN    | 110      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 868   | 562 | 156 | 147 | 3 |         |       |

- Molecule 39 is a protein called Small ribosomal subunit protein mS40.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 39  | AO    | 193      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1592  | 1014 | 294 | 277 | 7 |         |       |

- Molecule 40 is a protein called Small ribosomal subunit protein bS18m.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 40  | AP    | 97       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 781   | 501 | 134 | 138 | 8 |         |       |

- Molecule 41 is a protein called MRPS21 isoform 1.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 41  | AQ    | 87       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 744   | 460 | 150 | 126 | 8 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment     | Reference      |
|-------|---------|----------|--------|-------------|----------------|
| AQ    | 1       | ACE      | -      | acetylation | UNP A0A2J8VEN6 |

- Molecule 42 is a protein called Small ribosomal subunit protein mS22.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 42  | AR    | 295      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2409  | 1533 | 413 | 455 | 8 |         |       |

- Molecule 43 is a protein called Small ribosomal subunit protein mS23.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 43  | AS    | 135      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1111  | 716 | 198 | 196 | 1 |         |       |

- Molecule 44 is a protein called Small ribosomal subunit protein mS25.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 44  | AT    | 168      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1371  | 877 | 239 | 244 | 11 |         |       |

- Molecule 45 is a protein called Small ribosomal subunit protein mS26.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 45  | AU    | 176      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1488  | 916 | 301 | 267 | 4 |         |       |

- Molecule 46 is a protein called Small ribosomal subunit protein mS27.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 46  | AV    | 362      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2969  | 1904 | 495 | 558 | 12 |         |       |

- Molecule 47 is a protein called Small ribosomal subunit protein bS1m.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 47  | AW    | 100      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 789   | 498 | 141 | 146 | 4 |         |       |

- Molecule 48 is a protein called Small ribosomal subunit protein mS29.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 48  | AX    | 352      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2849  | 1822 | 499 | 517 | 11 |         |       |

- Molecule 49 is a protein called Small ribosomal subunit protein mS31.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 49  | AY    | 120      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1016  | 657 | 167 | 190 | 2 |         |       |

- Molecule 50 is a protein called Small ribosomal subunit protein mS33.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 50  | AZ    | 100      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 839   | 534 | 153 | 148 | 4 |         |       |

- Molecule 51 is a protein called Small ribosomal subunit protein mS34.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 51  | A0    | 215      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1787  | 1130 | 339 | 313 | 5 |         |       |

- Molecule 52 is a protein called Small ribosomal subunit protein mS35.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 52  | A1    | 277      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2245  | 1424 | 382 | 428 | 11 |         |       |

- Molecule 53 is a protein called Small ribosomal subunit protein mS37.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 53  | A2    | 118      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 935   | 579 | 182 | 166 | 8 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment     | Reference  |
|-------|---------|----------|--------|-------------|------------|
| A2    | 1       | ACE      | -      | acetylation | UNP Q96BP2 |

- Molecule 54 is a protein called Small ribosomal subunit protein mS38.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 54  | A3    | 70       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 625   | 401 | 134 | 89 | 1 |         |       |

- Molecule 55 is a protein called Small ribosomal subunit protein mS39.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 55  | A4    | 533      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4329  | 2780 | 730 | 793 | 26 |         |       |

- Molecule 56 is a RNA chain called P/P-tRNA.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 56  | Ax    | 65       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1378  | 617 | 242 | 454 | 65 |         |       |

- Molecule 57 is a RNA chain called mRNA.

| Mol | Chain | Residues | Atoms |    |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|-------|
| 57  | Az    | 8        | Total | C  | N  | O  | P | 0       | 0     |
|     |       |          | 167   | 75 | 25 | 59 | 8 |         |       |

- Molecule 58 is a protein called Large ribosomal subunit protein bL32m.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 58  | 0     | 110      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 898   | 554 | 176 | 162 | 6 |         |       |

- Molecule 59 is a protein called Large ribosomal subunit protein bL33m.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 59  | 1     | 53       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 440   | 281 | 84 | 73 | 2 |         |       |

- Molecule 60 is a protein called Large ribosomal subunit protein bL34m.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 60  | 2     | 46       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 377   | 233 | 83 | 60 | 1 |         |       |

- Molecule 61 is a protein called Large ribosomal subunit protein bL35m.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 61  | 3     | 95       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 832   | 539 | 162 | 128 | 3 |         |       |

- Molecule 62 is a protein called Large ribosomal subunit protein bL36m.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 62  | 4     | 38       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 342   | 217 | 72 | 49 | 4 |         |       |

- Molecule 63 is a protein called Large ribosomal subunit protein mL37.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 63  | 5     | 394      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3210  | 2073 | 560 | 566 | 11 |         |       |

- Molecule 64 is a protein called Large ribosomal subunit protein mL38.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 64  | 6     | 354      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2948  | 1881 | 525 | 533 | 9 |         |       |

- Molecule 65 is a protein called Large ribosomal subunit protein mL39.



| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 65  | 7     | 294      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2390  | 1529 | 405 | 438 | 18 |         |       |

- Molecule 66 is a protein called Large ribosomal subunit protein mL40.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 66  | 8     | 140      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1184  | 755 | 208 | 219 | 2 |         |       |

- Molecule 67 is a protein called Large ribosomal subunit protein mL41.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 67  | 9     | 124      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 997   | 644 | 170 | 181 | 2 |         |       |

- Molecule 68 is a protein called Large ribosomal subunit protein mL42.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 68  | a     | 100      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 840   | 529 | 152 | 154 | 5 |         |       |

- Molecule 69 is a protein called Large ribosomal subunit protein mL43.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 69  | b     | 151      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1196  | 744 | 231 | 218 | 3 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment     | Reference  |
|-------|---------|----------|--------|-------------|------------|
| b     | 1       | ACE      | -      | acetylation | UNP Q8N983 |

- Molecule 70 is a protein called Large ribosomal subunit protein mL44.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 70  | c     | 286      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2299  | 1470 | 397 | 423 | 9 |         |       |

- Molecule 71 is a protein called Large ribosomal subunit protein mL45.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 71  | d     | 241      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1985  | 1273 | 340 | 359 | 13 |         |       |

- Molecule 72 is a protein called Large ribosomal subunit protein mL46.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 72  | e     | 238      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1931  | 1222 | 339 | 364 | 6 |         |       |

- Molecule 73 is a protein called Large ribosomal subunit protein mL48.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 73  | f     | 157      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1252  | 799 | 207 | 242 | 4 |         |       |

- Molecule 74 is a protein called Large ribosomal subunit protein mL49.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 74  | g     | 134      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1113  | 719 | 193 | 199 | 2 |         |       |

- Molecule 75 is a protein called Large ribosomal subunit protein mL50.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 75  | h     | 110      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 895   | 568 | 156 | 168 | 3 |         |       |

- Molecule 76 is a protein called Large ribosomal subunit protein mL51.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 76  | i     | 97       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 828   | 532 | 165 | 127 | 4 |         |       |

- Molecule 77 is a protein called Large ribosomal subunit protein mL52.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 77  | j     | 94       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 745   | 463 | 144 | 136 | 2 |         |       |

- Molecule 78 is a protein called Large ribosomal subunit protein mL53.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 78  | k     | 95       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 738   | 459 | 142 | 132 | 5 |         |       |

- Molecule 79 is a protein called Large ribosomal subunit protein mL54.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 79  | l     | 82       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 688   | 437 | 120 | 128 | 3 |         |       |

- Molecule 80 is a protein called Large ribosomal subunit protein mL55.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 80  | m     | 92       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 791   | 488 | 159 | 142 | 2 |         |       |

- Molecule 81 is a protein called Large ribosomal subunit protein mL63.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 81  | o     | 94       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 798   | 501 | 165 | 129 | 3 |         |       |

- Molecule 82 is a protein called Large ribosomal subunit protein mL62.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 82  | p     | 143      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1179  | 735 | 222 | 218 | 4 |         |       |

- Molecule 83 is a protein called Large ribosomal subunit protein mL64.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 83  | q     | 133      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1120  | 697 | 220 | 198 | 5 |         |       |

- Molecule 84 is a protein called Large ribosomal subunit protein mL66.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 84  | r     | 162      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1322  | 839 | 252 | 223 | 8 |         |       |

- Molecule 85 is a protein called Large ribosomal subunit protein mL65.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 85  | s     | 383      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3134  | 2010 | 556 | 554 | 14 |         |       |

- Molecule 86 is a protein called Large ribosomal subunit protein bL12m.

| Mol | Chain | Residues | Atoms |    |    |    | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|-------|
| 86  | t     | 11       | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 72    | 44 | 12 | 16 |         |       |

- Molecule 87 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |     | AltConf |
|-----|-------|----------|-------|-----|---------|
| 87  | A     | 138      | Total | Mg  | 0       |
|     |       |          | 138   | 138 |         |
| 87  | D     | 2        | Total | Mg  | 0       |
|     |       |          | 2     | 2   |         |
| 87  | E     | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 87  | AA    | 63       | Total | Mg  | 0       |
|     |       |          | 63    | 63  |         |
| 87  | AB    | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 87  | AX    | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 87  | A3    | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 87  | g     | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |

- Molecule 88 is POTASSIUM ION (CCD ID: K) (formula: K).

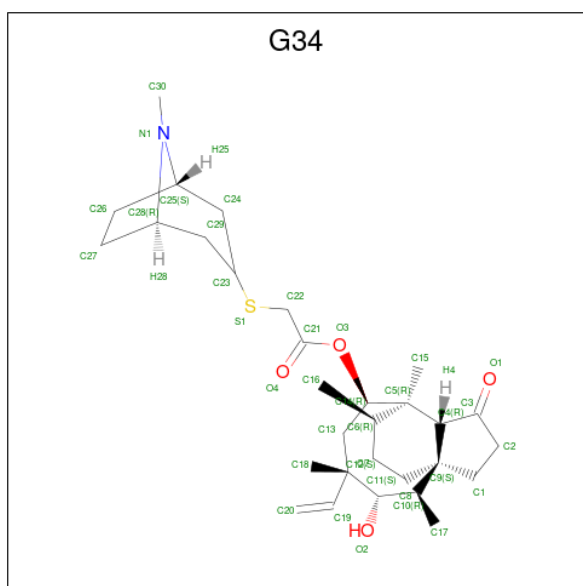
| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 88  | A     | 29       | Total | K  | 0       |
|     |       |          | 29    | 29 |         |
| 88  | D     | 1        | Total | K  | 0       |
|     |       |          | 1     | 1  |         |
| 88  | M     | 1        | Total | K  | 0       |
|     |       |          | 1     | 1  |         |
| 88  | W     | 1        | Total | K  | 0       |
|     |       |          | 1     | 1  |         |
| 88  | AA    | 18       | Total | K  | 0       |
|     |       |          | 18    | 18 |         |

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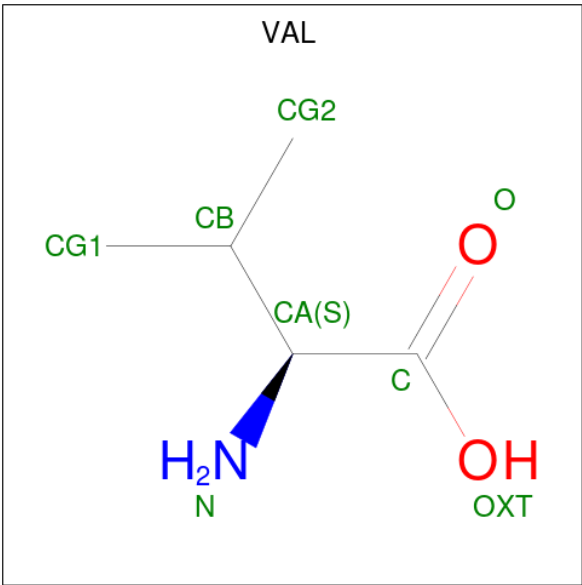
| Mol | Chain | Residues | Atoms |   | AltConf |
|-----|-------|----------|-------|---|---------|
| 88  | 6     | 1        | Total | K | 0       |
|     |       |          | 1     | 1 |         |
| 88  | i     | 1        | Total | K | 0       |
|     |       |          | 1     | 1 |         |
| 88  | o     | 1        | Total | K | 0       |
|     |       |          | 1     | 1 |         |

- Molecule 89 is Retapamulin (CCD ID: G34) (formula:  $C_{30}H_{47}NO_4S$ ) (labeled as "Ligand of Interest" by depositor).



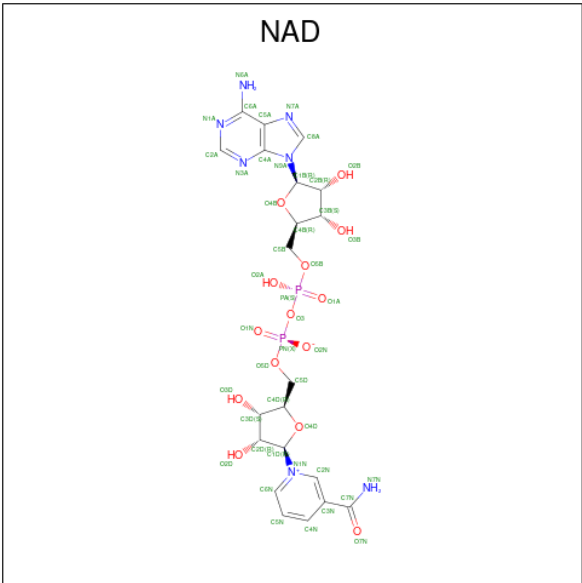
| Mol | Chain | Residues | Atoms |    |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 89  | A     | 1        | Total | C  | N | O | S | 0       |
|     |       |          | 36    | 30 | 1 | 4 | 1 |         |

- Molecule 90 is VALINE (CCD ID: VAL) (formula:  $C_5H_{11}NO_2$ ).



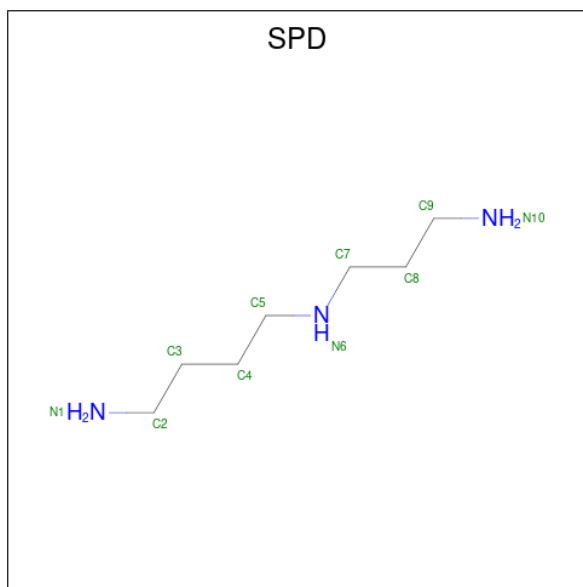
| Mol | Chain | Residues | Atoms |   |   |   | AltConf |
|-----|-------|----------|-------|---|---|---|---------|
| 90  | B     | 1        | Total | C | N | O | 0       |
|     |       |          | 7     | 5 | 1 | 1 |         |

- Molecule 91 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: C<sub>21</sub>H<sub>27</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>).



| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 91  | AA    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 44    | 21 | 7 | 14 | 2 |         |

- Molecule 92 is SPERMIDINE (CCD ID: SPD) (formula: C<sub>7</sub>H<sub>19</sub>N<sub>3</sub>).



| Mol | Chain | Residues | Atoms |   |   | AltConf |
|-----|-------|----------|-------|---|---|---------|
| 92  | AA    | 1        | Total | C | N | 0       |
|     |       |          | 10    | 7 | 3 |         |

- Molecule 93 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 93  | AO    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 93  | 0     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 93  | 4     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 94 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).



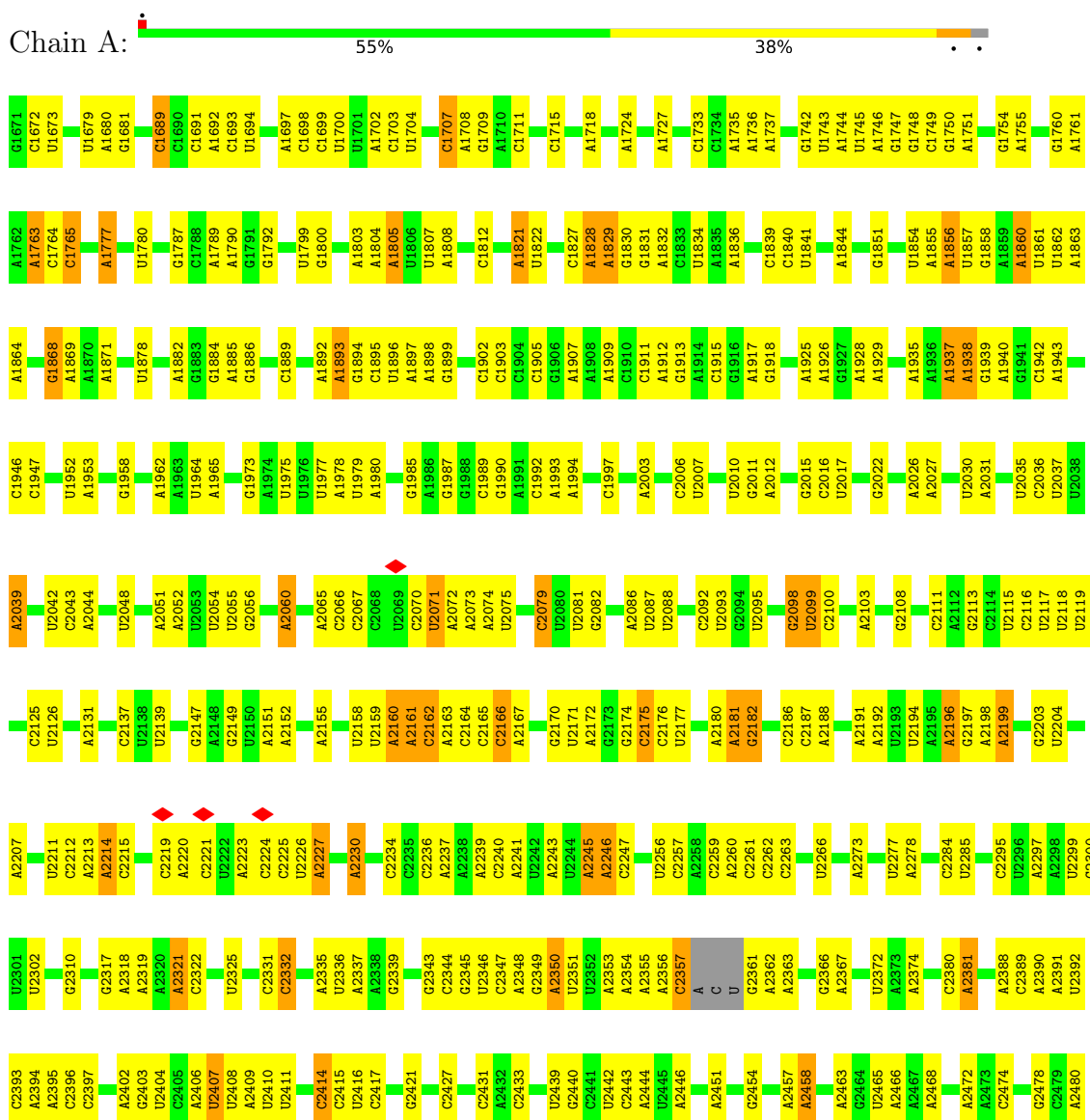


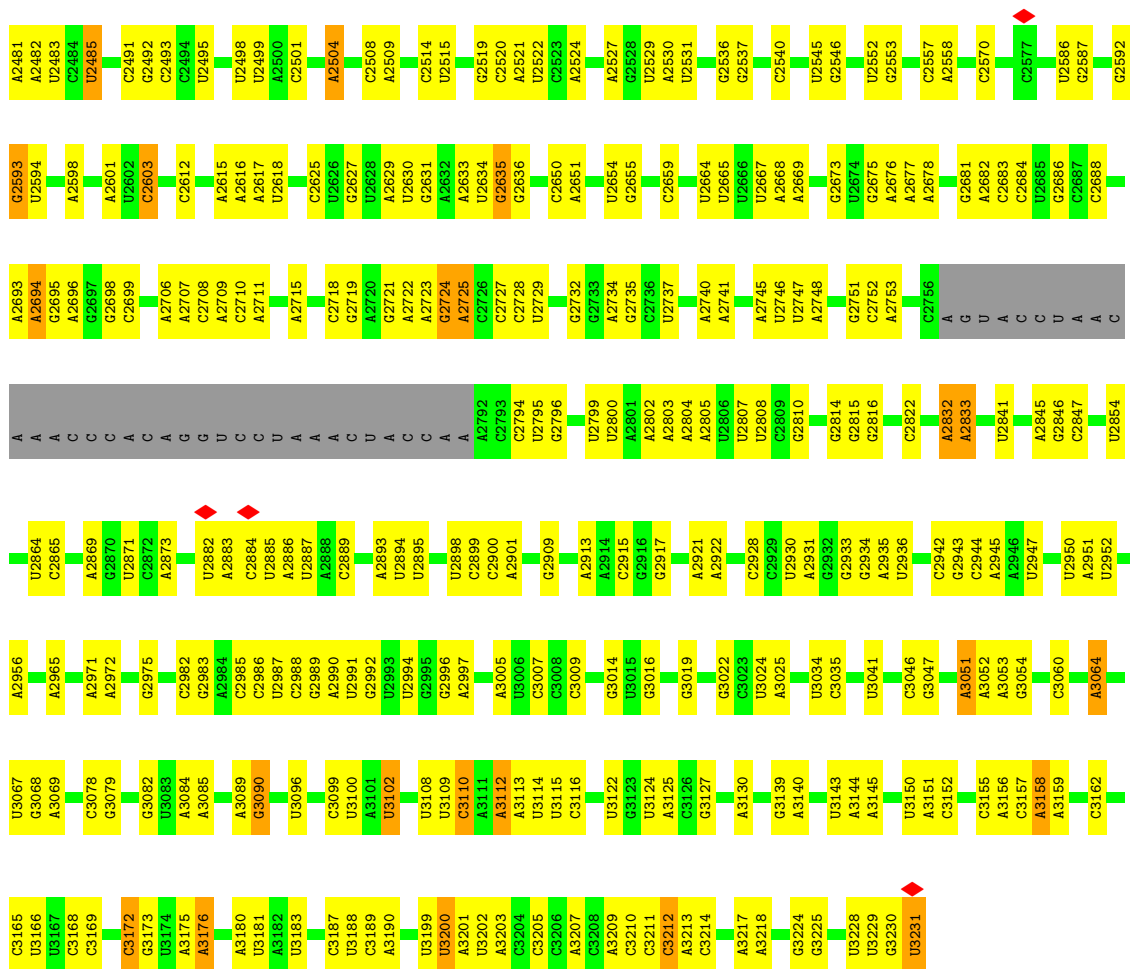


### 3 Residue-property plots

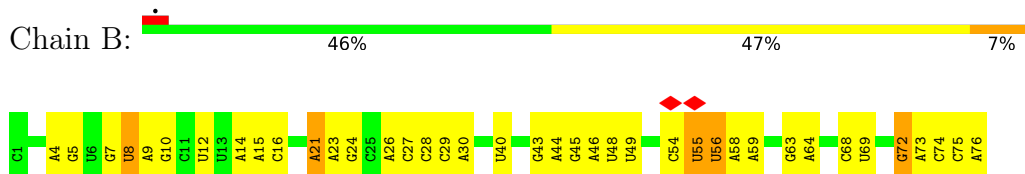
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 16S mitochondrial rRNA

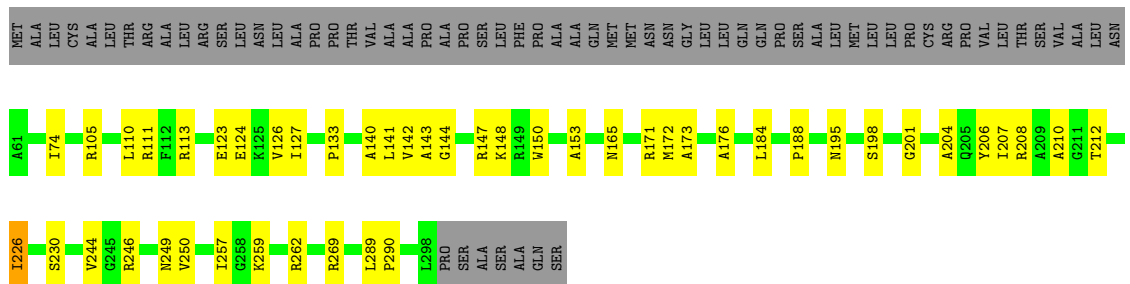




• Molecule 2: mitochondrial tRNA<sup>Val</sup>



• Molecule 3: Large ribosomal subunit protein uL2m



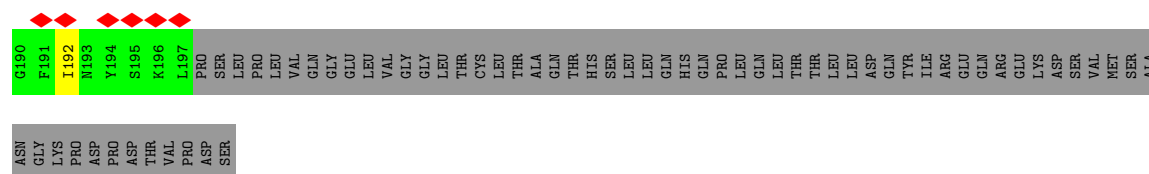
• Molecule 4: Large ribosomal subunit protein uL3m

|      |     |     |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |     |     |     |     |     |     |     |
|------|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|
| A348 | P84 | R96 | T111 | K112 | D113 | K141 | G148 | G149 | K150 | R154 | F155 | R156 | L170 | K173 | Q174 | H197 | T210 | F215 | M219 | K220 | R221 | W222 | G232 | A244 | I248 | K256 | M257 | G262 | R266 | R275 | V285 | P290 | K298 | G323 | D331 | T345 |     |     |     |     |     |     |     |
| MET  | PRO | TRP | ARG  | LEU  | LEU  | THR  | GLN  | VAL  | GLY  | ALA  | GLN  | VAL  | LEU  | GLY  | ARG  | LEU  | GLY  | ASP  | ASN  | ARG  | THR  | HIS  | ILE  | TRP  | LEU  | PHE  | VAL  | ARG  | GLY  | LEU  | HIS  | GLY  | K44  | T47  | D50  | L64  | D69 | K76 | L77 | C78 | P79 | L80 | K81 |

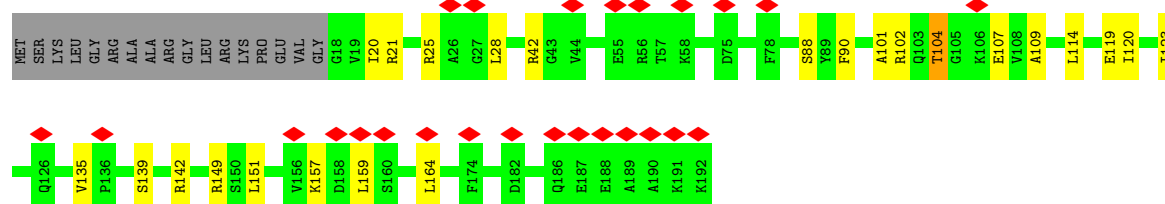
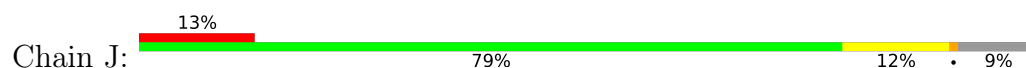
- [illegible]

- | Position | Residue | Conservation | Annotations |
|----------|---------|--------------|-------------|
| 1        | PHE     | 0.00         |             |
| 2        | GLU     | 0.00         |             |
| 3        | LYS     | 0.00         |             |
| 4        | PRO     | 0.00         |             |
| 5        | LYS     | 0.00         |             |
| 6        | THR     | 0.00         |             |
| 7        | LYS     | 0.00         |             |
| 8        | ARG     | 0.00         |             |
| 9        | TYR     | 0.00         |             |
| 10       | LYS     | 0.00         |             |
| 11       | TYR     | 0.00         |             |
| 12       | TRP     | 0.00         |             |
| 13       | LEU     | 0.00         |             |
| 14       | ALA     | 0.00         |             |
| 15       | GLN     | 0.00         |             |
| 16       | ALA     | 0.00         |             |
| 17       | ALA     | 0.00         |             |
| 18       | LYS     | 0.00         |             |
| 19       | ALA     | 0.00         |             |
| 20       | MET     | 0.00         |             |
| 21       | PRO     | 0.00         |             |
| 22       | THR     | 0.00         |             |
| 23       | SER     | 0.00         |             |
| 24       | PRO     | 0.00         |             |
| 25       | GLN     | 0.00         |             |
| 26       | ILE     | 0.00         |             |
| 27       | VAL     | 0.00         |             |
| 28       | VAL     | 0.00         |             |
| 29       | VAL     | 0.00         |             |
| 30       | VAL     | 0.00         |             |
| 31       | VAL     | 0.00         |             |
| 32       | VAL     | 0.00         |             |
| 33       | VAL     | 0.00         |             |
| 34       | VAL     | 0.00         |             |
| 35       | VAL     | 0.00         |             |
| 36       | VAL     | 0.00         |             |
| 37       | VAL     | 0.00         |             |
| 38       | VAL     | 0.00         |             |
| 39       | VAL     | 0.00         |             |
| 40       | VAL     | 0.00         |             |
| 41       | VAL     | 0.00         |             |
| 42       | VAL     | 0.00         |             |
| 43       | VAL     | 0.00         |             |
| 44       | VAL     | 0.00         |             |
| 45       | VAL     | 0.00         |             |
| 46       | VAL     | 0.00         |             |
| 47       | VAL     | 0.00         |             |
| 48       | VAL     | 0.00         |             |
| 49       | VAL     | 0.00         |             |
| 50       | VAL     | 0.00         |             |
| 51       | VAL     | 0.00         |             |
| 52       | VAL     | 0.00         |             |
| 53       | VAL     | 0.00         |             |
| 54       | VAL     | 0.00         |             |
| 55       | VAL     | 0.00         |             |
| 56       | VAL     | 0.00         |             |
| 57       | VAL     | 0.00         |             |
| 58       | VAL     | 0.00         |             |
| 59       | VAL     | 0.00         |             |
| 60       | VAL     | 0.00         |             |
| 61       | VAL     | 0.00         |             |
| 62       | VAL     | 0.00         |             |
| 63       | VAL     | 0.00         |             |
| 64       | VAL     | 0.00         |             |
| 65       | VAL     | 0.00         |             |
| 66       | VAL     | 0.00         |             |
| 67       | VAL     | 0.00         |             |
| 68       | VAL     | 0.00         |             |
| 69       | VAL     | 0.00         |             |
| 70       | VAL     | 0.00         |             |
| 71       | VAL     | 0.00         |             |
| 72       | VAL     | 0.00         |             |
| 73       | VAL     | 0.00         |             |
| 74       | VAL     | 0.00         |             |
| 75       | VAL     | 0.00         |             |
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| 77       | VAL     | 0.00         |             |
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| 79       | VAL     | 0.00         |             |
| 80       | VAL     | 0.00         |             |
| 81       | VAL     | 0.00         |             |
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| 83       | VAL     | 0.00         |             |
| 84       | VAL     | 0.00         |             |
| 85       | VAL     | 0.00         |             |
| 86       | VAL     | 0.00         |             |
| 87       | VAL     | 0.00         |             |
| 88       | VAL     | 0.00         |             |
| 89       | VAL     | 0.00         |             |
| 90       | VAL     | 0.00         |             |
| 91       | VAL     | 0.00         |             |
| 92       | VAL     | 0.00         |             |
| 93       | VAL     | 0.00         |             |
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| 95       | VAL     | 0.00         |             |
| 96       | VAL     | 0.00         |             |
| 97       | VAL     | 0.00         |             |
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| 103      | VAL     | 0.00         |             |
| 104      | VAL     | 0.00         |             |
| 105      | VAL     | 0.00         |             |
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| 108      | VAL     | 0.00         |             |
| 109      | VAL     | 0.00         |             |
| 110      | VAL     | 0.00         |             |
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| 112      | VAL     | 0.00         |             |
| 113      | VAL     | 0.00         |             |
| 114      | VAL     | 0.00         |             |
| 115      | VAL     | 0.00         |             |
| 116      | VAL     | 0.00         |             |
| 117      | VAL     | 0.00         |             |
| 118      | VAL     | 0.00         |             |
| 119      | VAL     | 0.00         |             |
| 120      | VAL     | 0.00         |             |
| 121      | VAL     | 0.00         |             |
| 122      | VAL     | 0.00         |             |
| 123      | VAL     | 0.00         |             |
| 124      | VAL     | 0.00         |             |
| 125      | VAL     | 0.00         |             |
| 126      | VAL     | 0.00         |             |
| 127      | VAL     | 0.00         |             |
| 128      | VAL     | 0.00         |             |
| 129      | VAL     | 0.00         |             |
| 130      |         |              |             |

- 
- Diagram illustrating a sequence of amino acids (top row) and their corresponding codons (bottom row). The sequence is divided into segments by vertical lines. Red diamonds indicate specific positions or relationships between the two rows.
- Amino Acid Sequence (Top Row):** MET, ALA, ALA, ALA, VAL, ALA, GLY, MET, MET, LEU, ARG, GLY, GLY, LEU, LEU, GLN, GLN, ALA, GLY, ARG, ARG, THR, THR, LEU, GLN, THR, VAL, ARG, ARG, THR, Q29.
- Codon Sequence (Bottom Row):** L116, H119, K120, I121, L122, M123, K124, L128, Q129, V130, D137, S138, K139, Y140, Q141, N142, L143, L146, F147, V148, M151, M152, L153, L154, V155, S156, E157, E158, P159, K160, V161, K162, E163, R166, I167, L168, R169, T170, F173, L176, L177, I181, D182, T184, L185, L186, S187, R188, R189.
- Red diamonds are positioned above the following amino acids: MET, ALA, VAL, MET, MET, ARG, GLY, GLY, LEU, LEU, GLN, GLN, ALA, GLY, ARG, ARG, THR, THR, LEU, GLN, THR, VAL, ARG, ARG, THR, Q29.



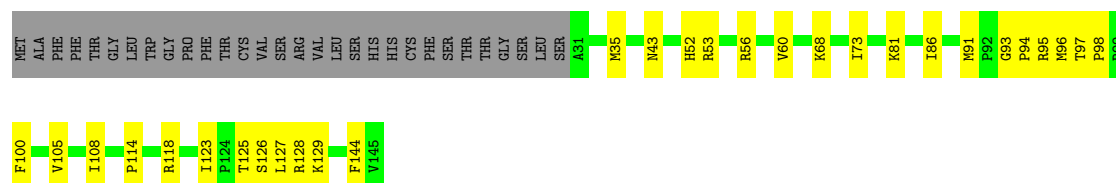
- Molecule 8: Large ribosomal subunit protein uL11m



- Molecule 9: Large ribosomal subunit protein uL13m



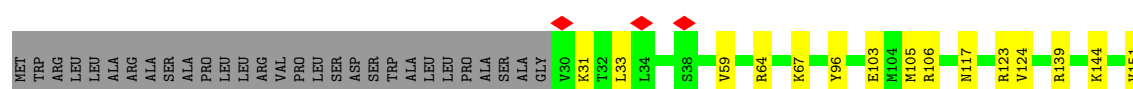
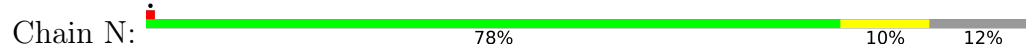
- Molecule 10: Large ribosomal subunit protein uL14m



- Molecule 11: Large ribosomal subunit protein uL15m

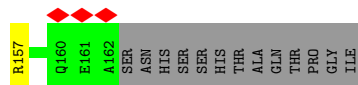


- Molecule 12: Large ribosomal subunit protein uL16m

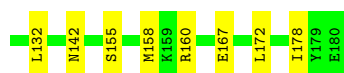
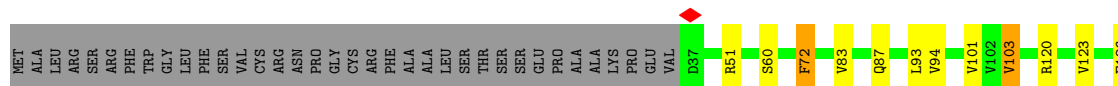




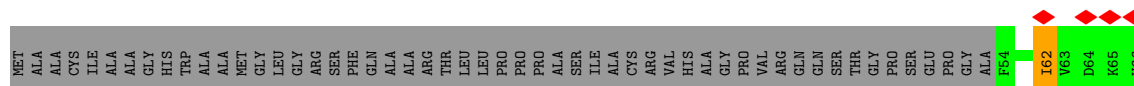
- Molecule 13: Large ribosomal subunit protein bL17m



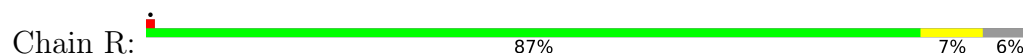
- Molecule 14: Large ribosomal subunit protein uL18m



- Molecule 15: Large ribosomal subunit protein bL19m

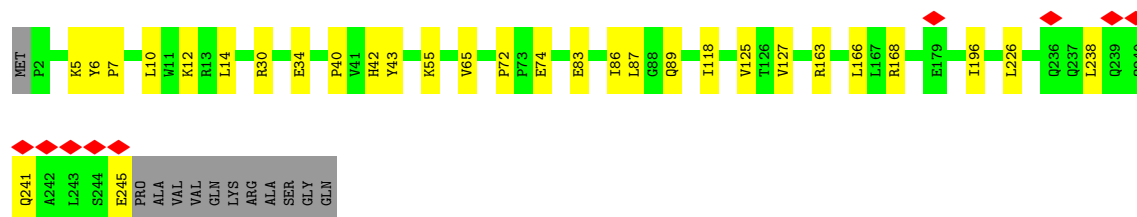


- Molecule 16: Large ribosomal subunit protein bL20m



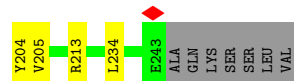
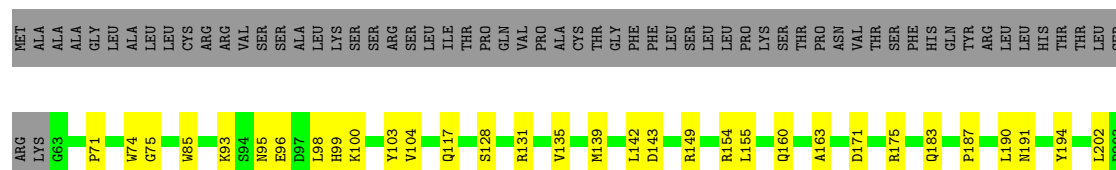
- Molecule 17: Large ribosomal subunit protein bL21m





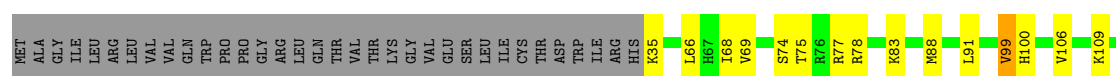
- Molecule 23: Large ribosomal subunit protein uL29m

Chain Y: 58% 14% 28%



- Molecule 24: Large ribosomal subunit protein uL30m

Chain Z: 64% 11% 24%



- Molecule 25: 12S mitochondrial rRNA

Chain AA: 56% 40%



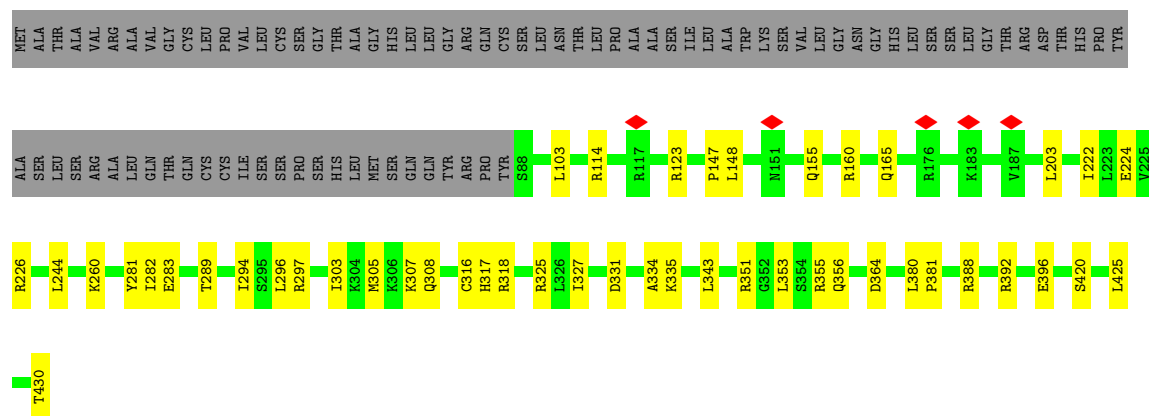


- Molecule 26: Small ribosomal subunit protein uS2m

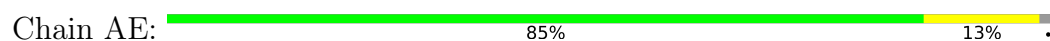
- Molecule 27: Small ribosomal subunit protein uS3m

- Molecule 28: Small ribosomal subunit protein uS5m

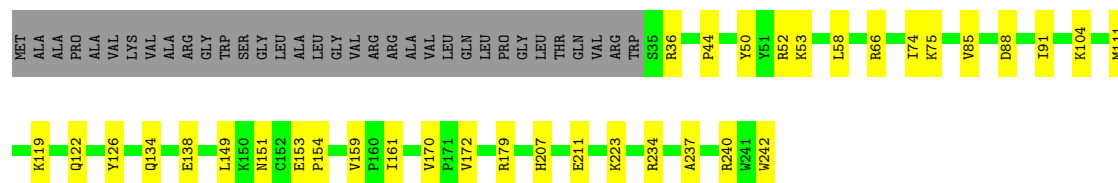




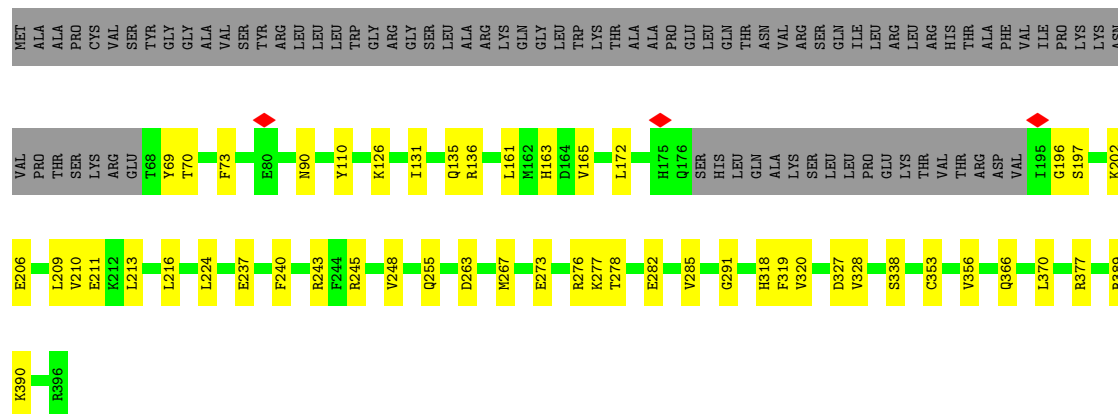
- Molecule 29: Small ribosomal subunit protein bS6m



- Molecule 30: Small ribosomal subunit protein uS7m

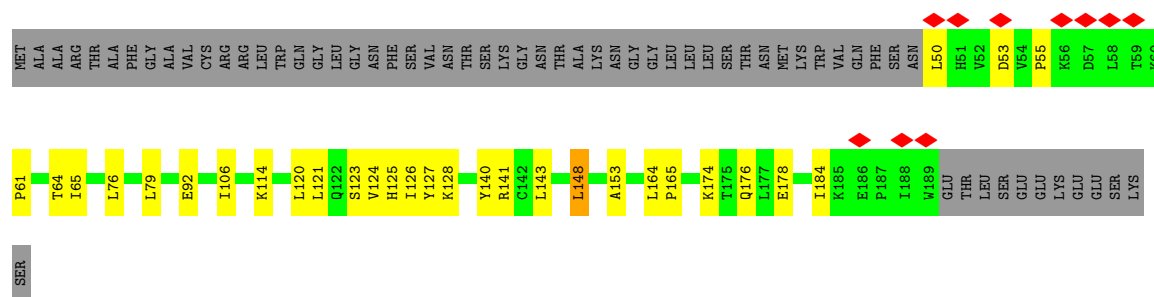


- Molecule 31: Small ribosomal subunit protein uS9m

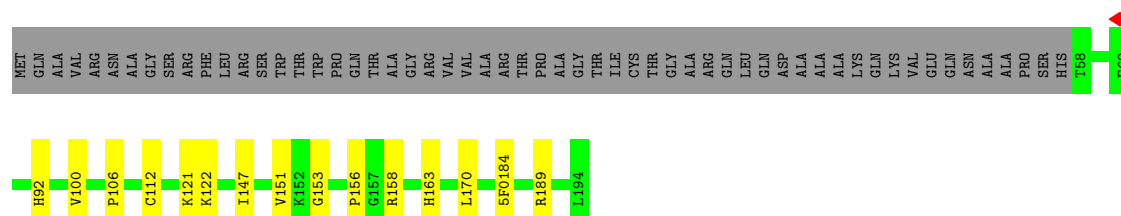


- Molecule 32: Small ribosomal subunit protein uS10m

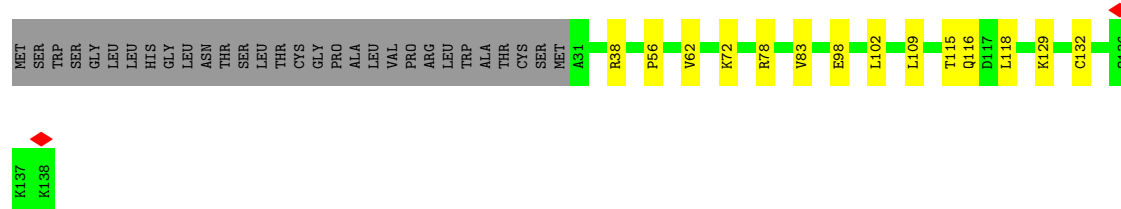




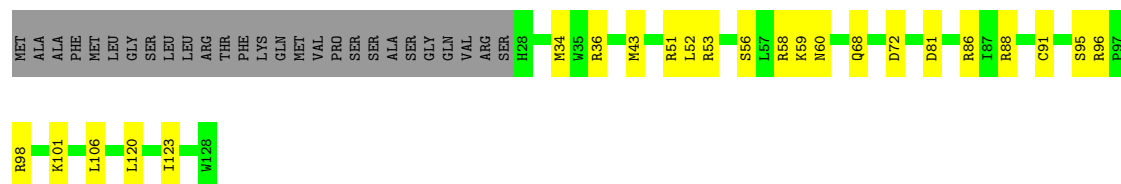
- Molecule 33: Small ribosomal subunit protein uS11m



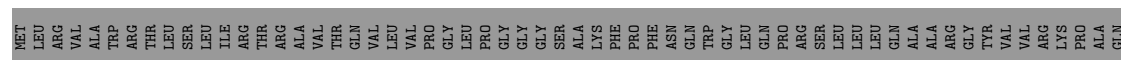
- Molecule 34: Small ribosomal subunit protein uS12m

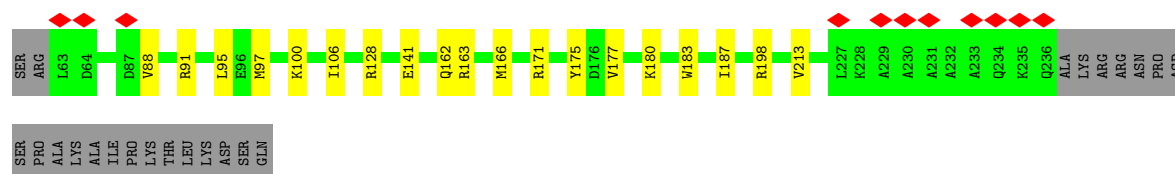


- Molecule 35: Small ribosomal subunit protein uS14m

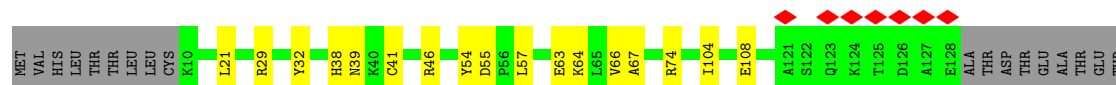
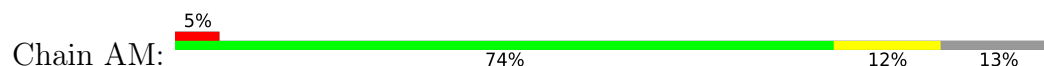


- Molecule 36: Small ribosomal subunit protein uS15m

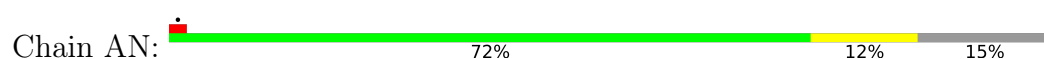




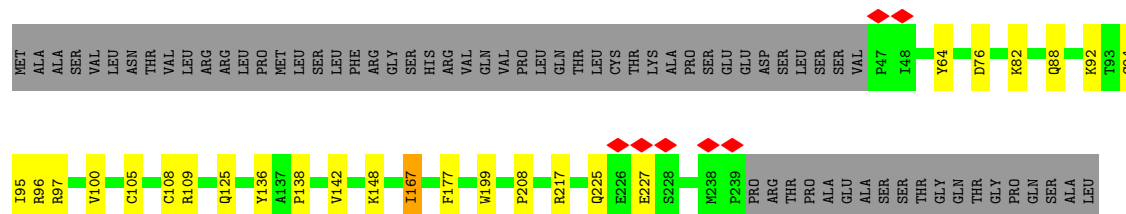
- Molecule 37: Small ribosomal subunit protein bS16m



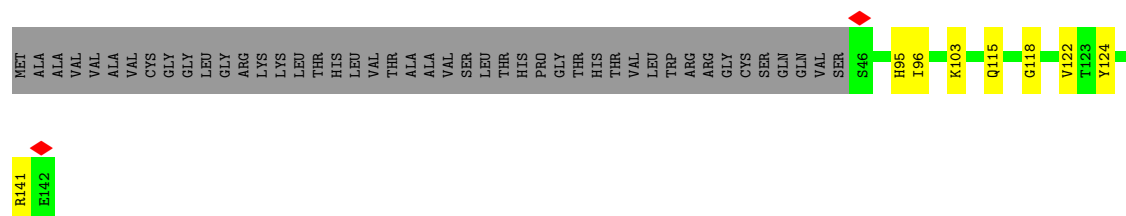
- Molecule 38: Small ribosomal subunit protein uS17m



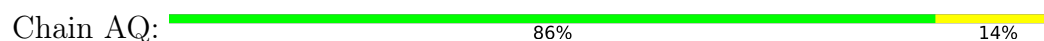
- Molecule 39: Small ribosomal subunit protein mS40



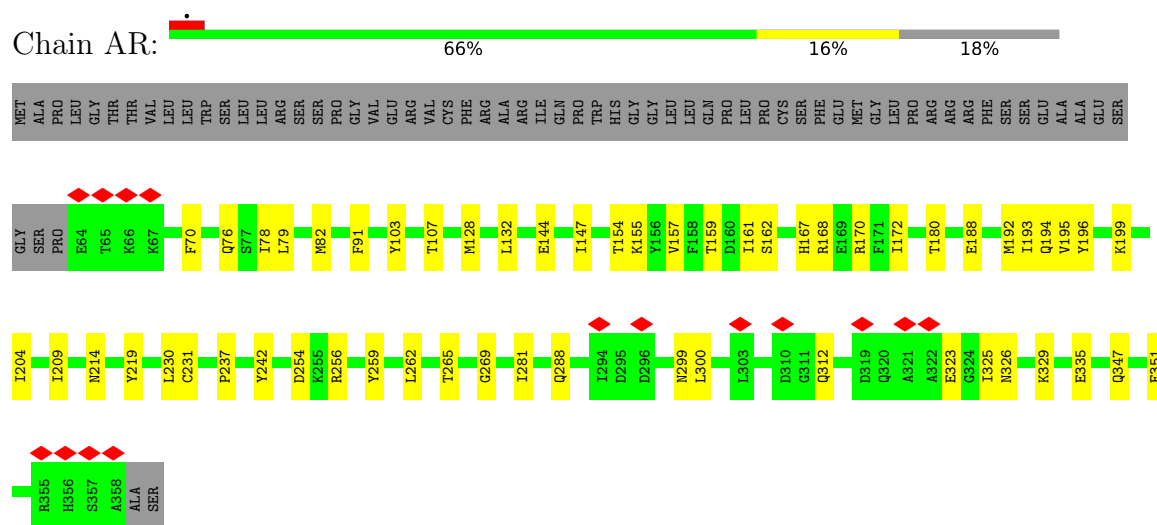
- Molecule 40: Small ribosomal subunit protein bS18m



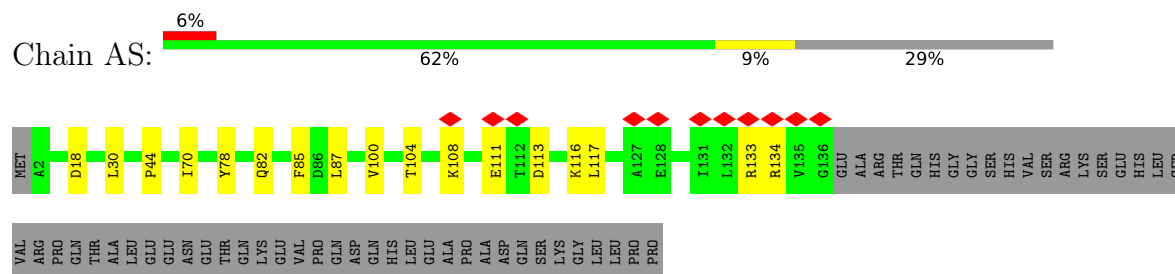
- Molecule 41: MRPS21 isoform 1



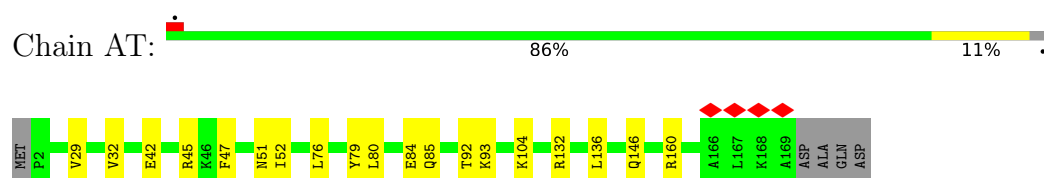
- Molecule 42: Small ribosomal subunit protein mS22



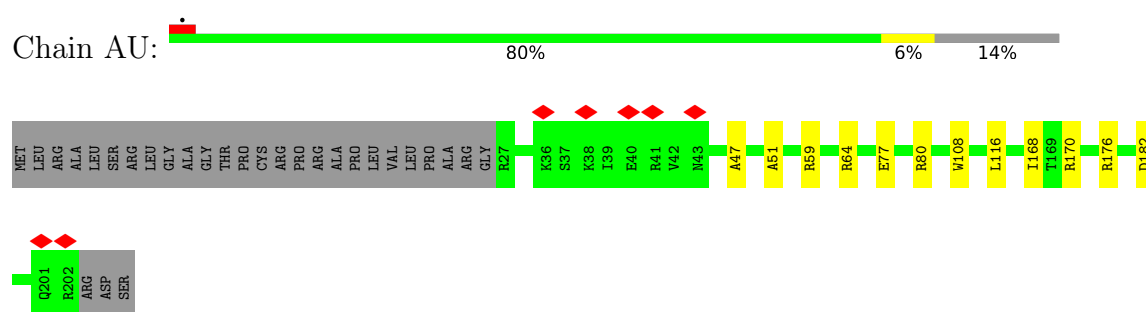
- Molecule 43: Small ribosomal subunit protein mS23



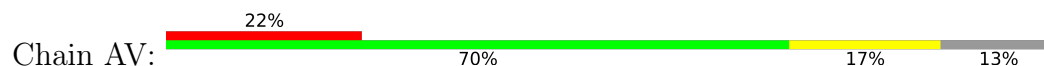
- Molecule 44: Small ribosomal subunit protein mS25

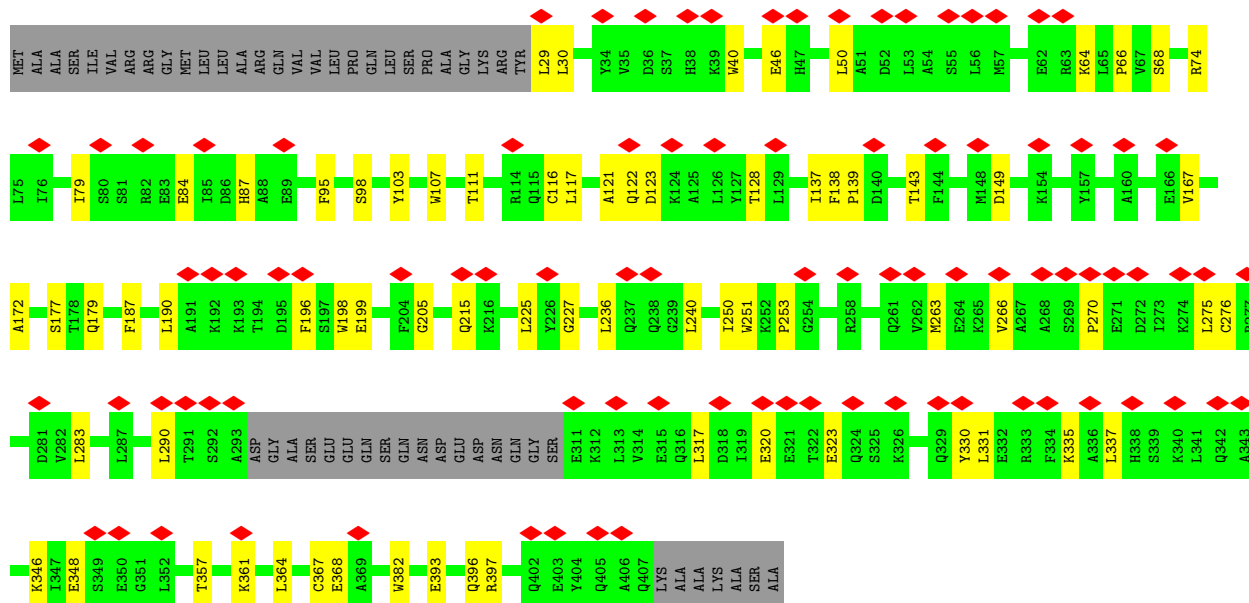


- Molecule 45: Small ribosomal subunit protein mS26



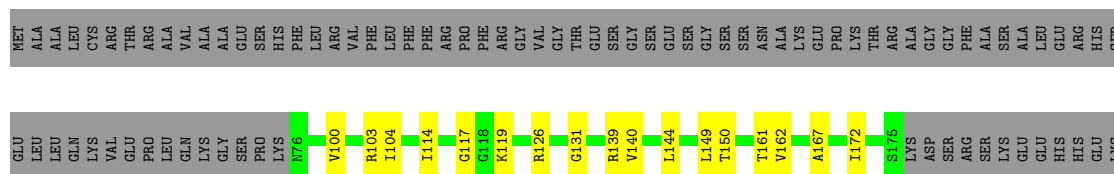
- Molecule 46: Small ribosomal subunit protein mS27





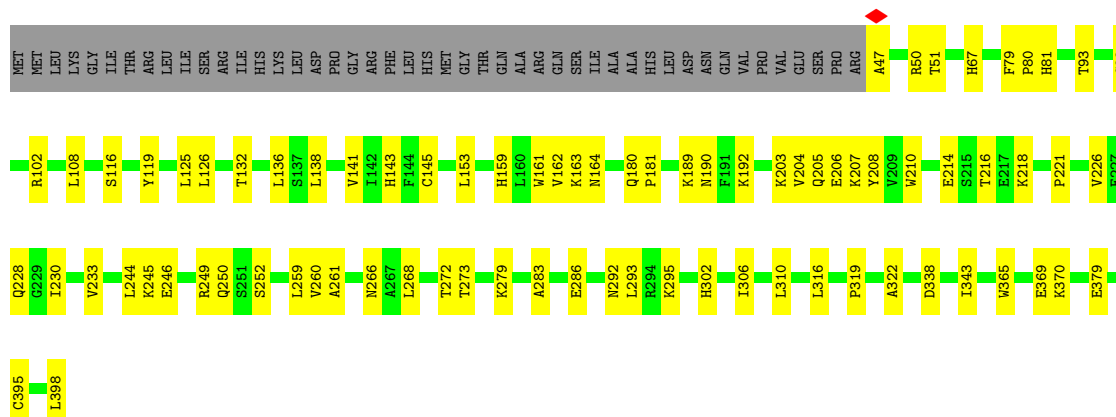
• Molecule 47: Small ribosomal subunit protein bS1m

Chain AW: 44% 9% 47%



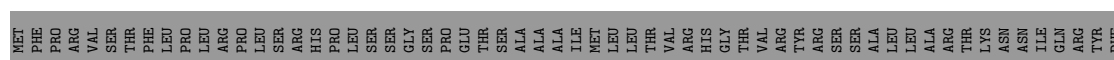
• Molecule 48: Small ribosomal subunit protein mS29

Chain AX: 68% 20% 12%



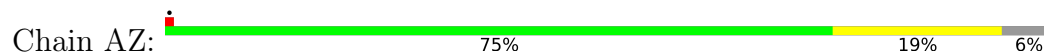
• Molecule 49: Small ribosomal subunit protein mS31

Chain AY: 29% 70%

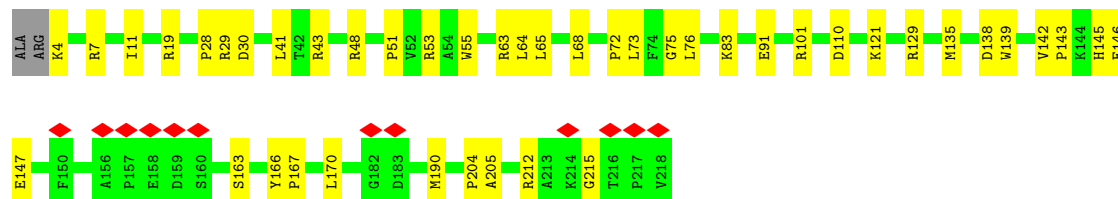
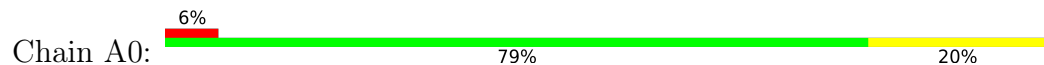




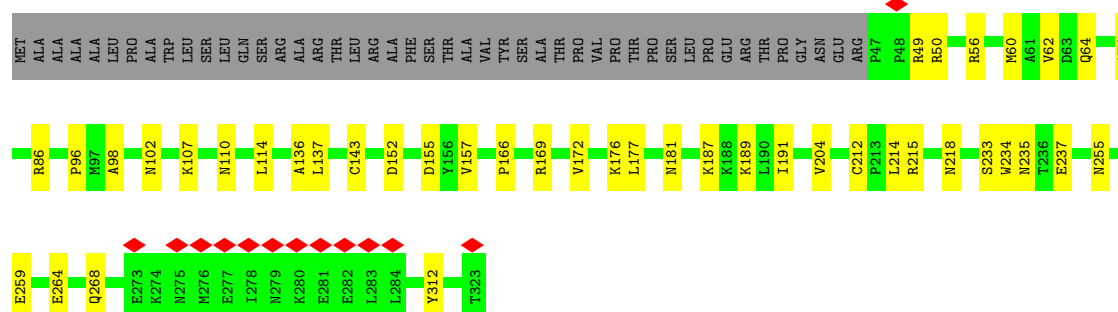
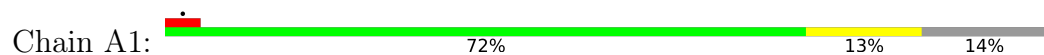
- Molecule 50: Small ribosomal subunit protein mS33



- Molecule 51: Small ribosomal subunit protein mS34



- Molecule 52: Small ribosomal subunit protein mS35

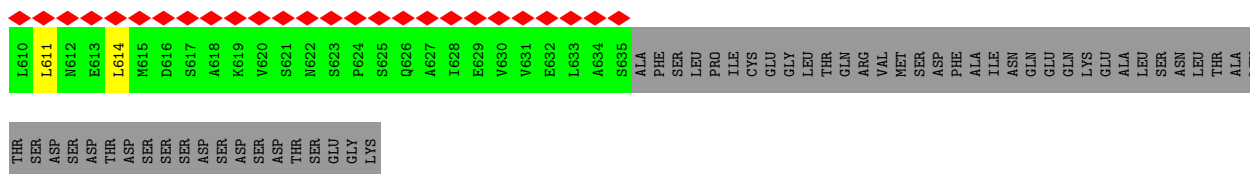


- Molecule 53: Small ribosomal subunit protein mS37









• Molecule 56: P/P-tRNA



• Molecule 57: mRNA



• Molecule 58: Large ribosomal subunit protein bL32m



• Molecule 59: Large ribosomal subunit protein bL33m

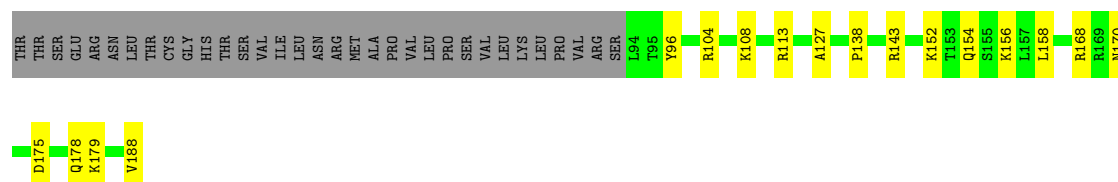


• Molecule 60: Large ribosomal subunit protein bL34m



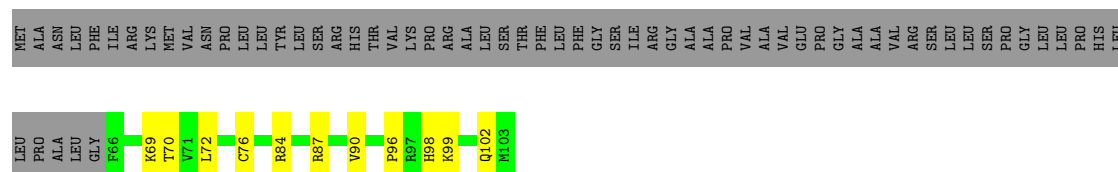
• Molecule 61: Large ribosomal subunit protein bL35m





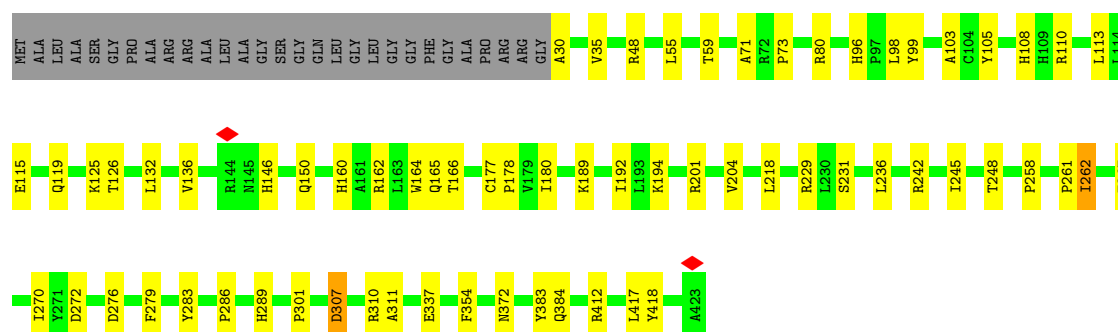
- Molecule 62: Large ribosomal subunit protein bL36m

Chain 4: 26% 11% 63%



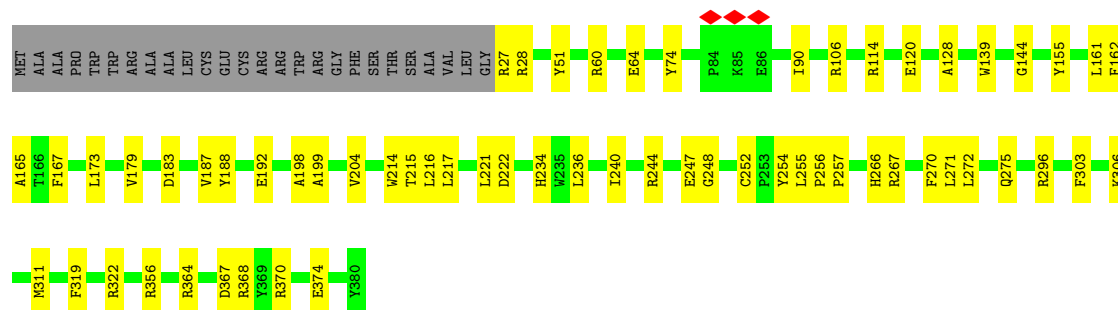
- Molecule 63: Large ribosomal subunit protein mL37

Chain 5: 77% 15% 7%



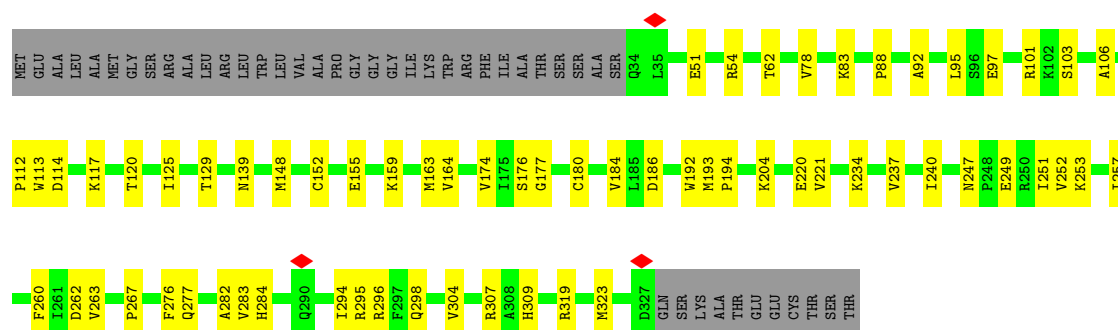
- Molecule 64: Large ribosomal subunit protein mL38

Chain 6: 77% 16% 7%

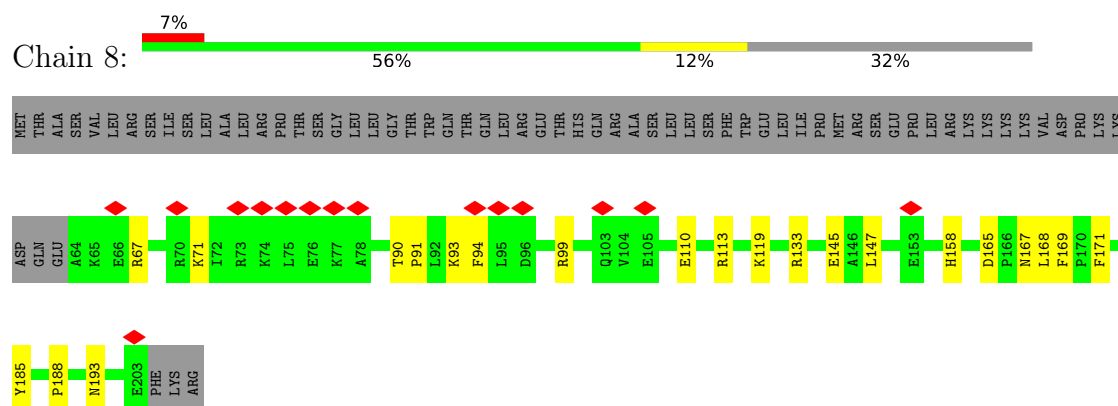


- Molecule 65: Large ribosomal subunit protein mL39

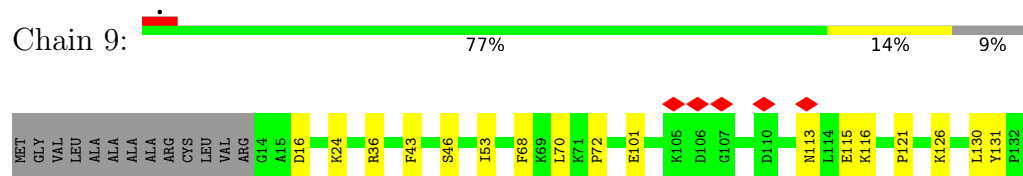
Chain 7: 68% 19% 13%



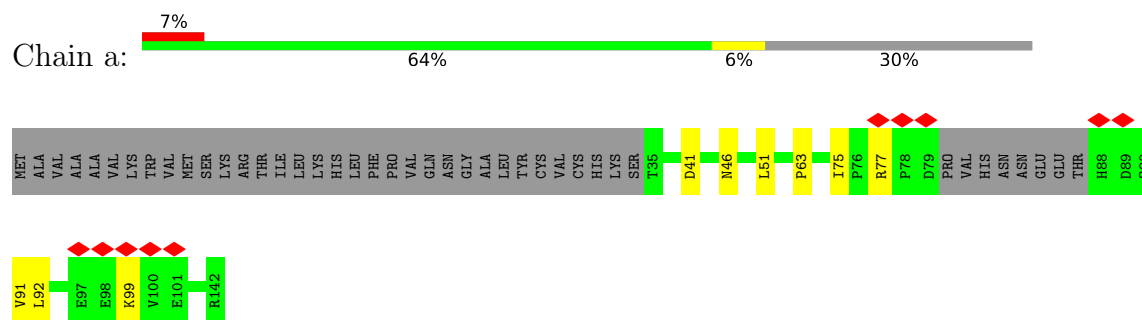
- Molecule 66: Large ribosomal subunit protein mL40



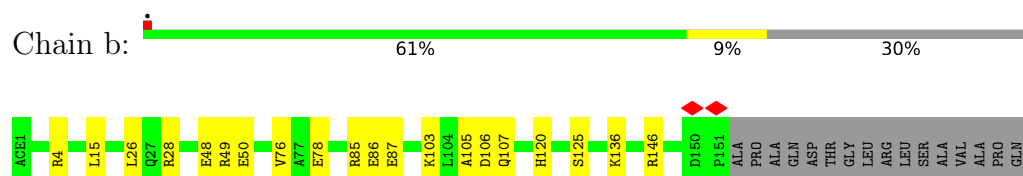
- Molecule 67: Large ribosomal subunit protein mL41



- Molecule 68: Large ribosomal subunit protein mL42

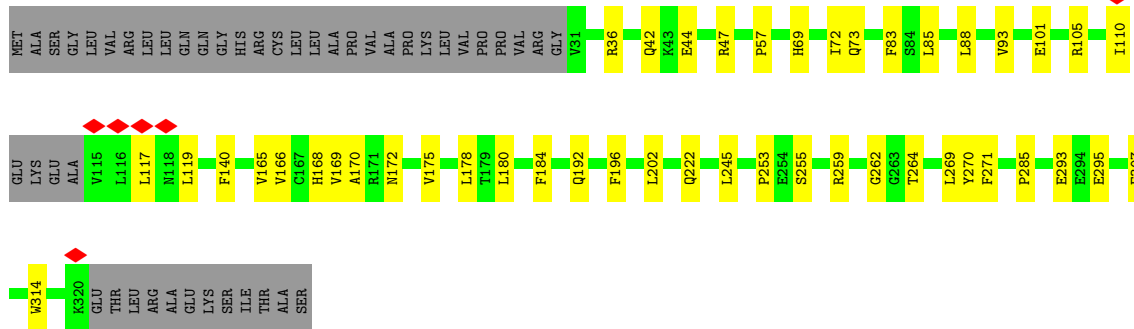


- Molecule 69: Large ribosomal subunit protein mL43



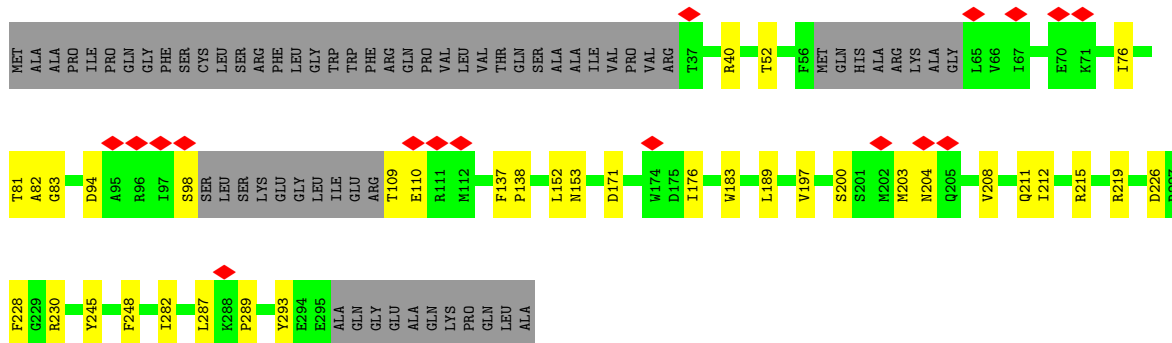
- Molecule 70: Large ribosomal subunit protein mL44

Chain c:



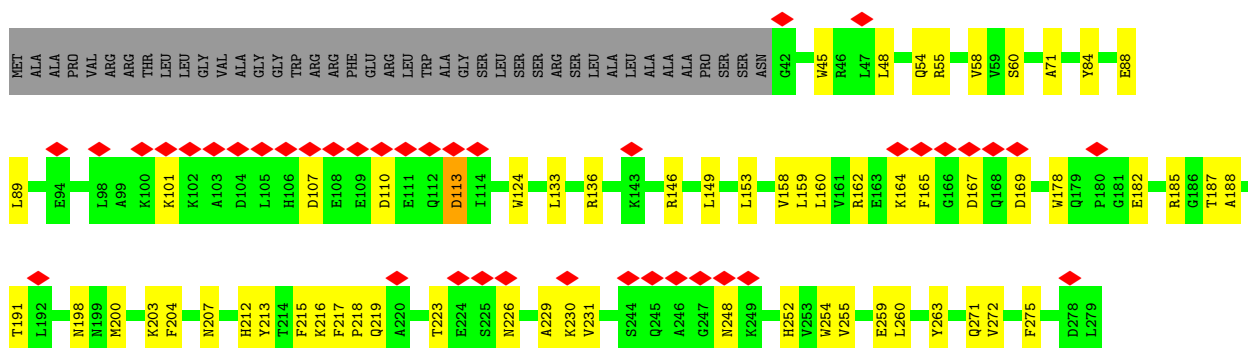
- Molecule 71: Large ribosomal subunit protein mL45

Chain d:



- Molecule 72: Large ribosomal subunit protein mL46

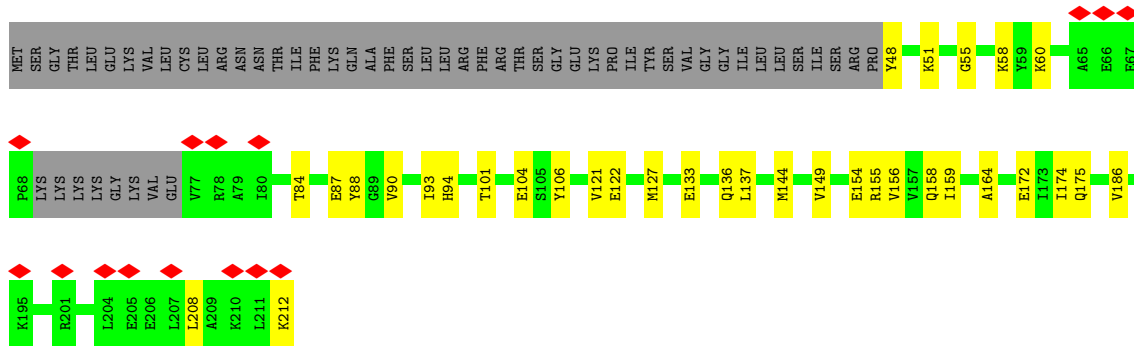
Chain e:



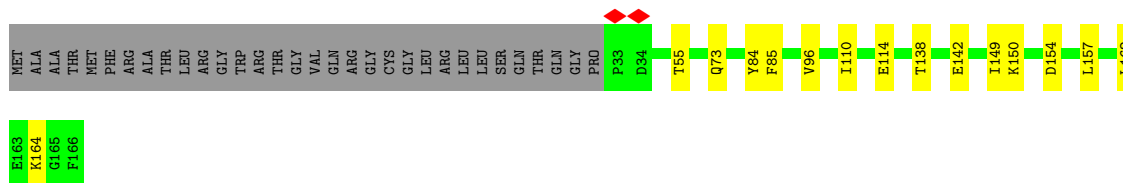
- Molecule 73: Large ribosomal subunit protein mL48

Chain f:

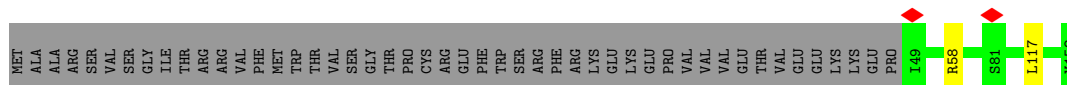




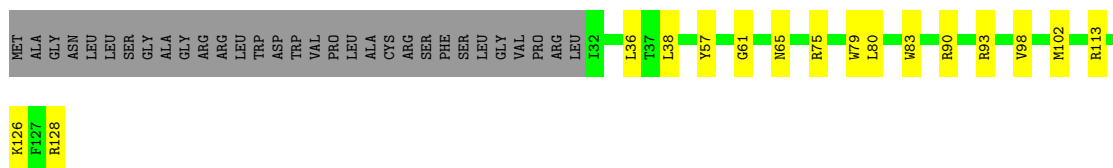
- Molecule 74: Large ribosomal subunit protein mL49



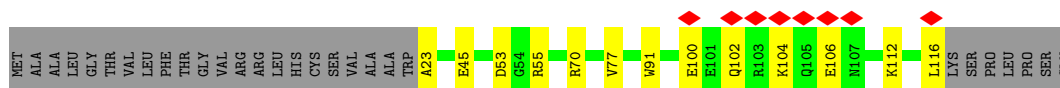
- Molecule 75: Large ribosomal subunit protein mL50



- Molecule 76: Large ribosomal subunit protein mL51



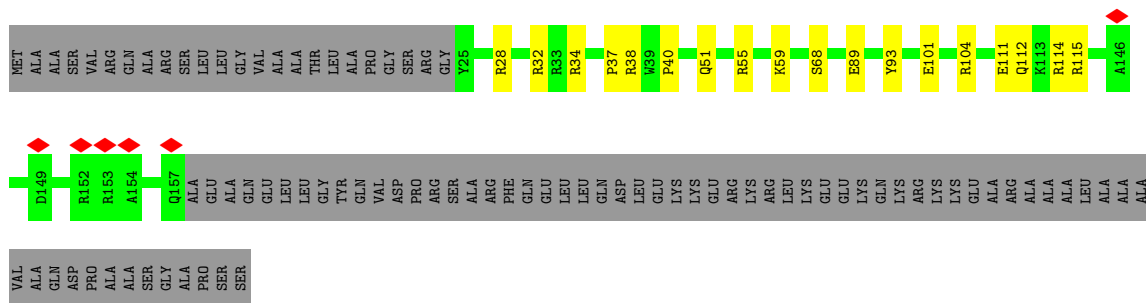
- Molecule 77: Large ribosomal subunit protein mL52



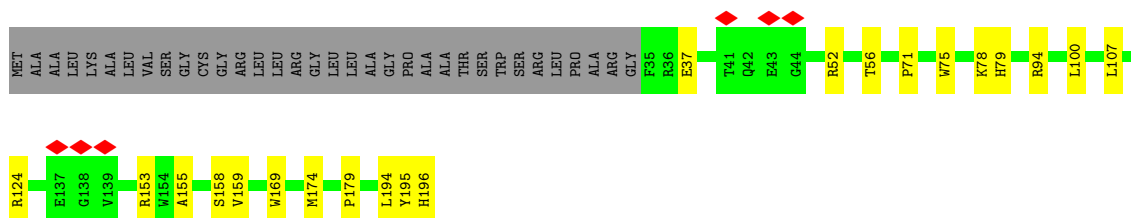
- Molecule 78: Large ribosomal subunit protein mL53



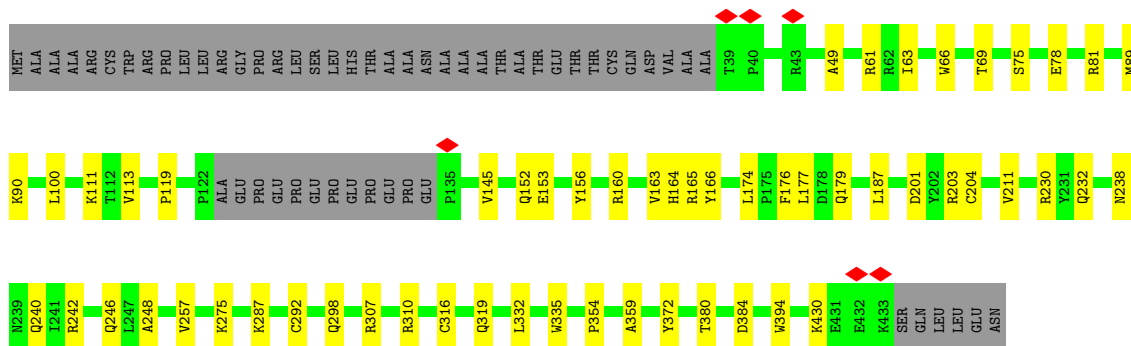




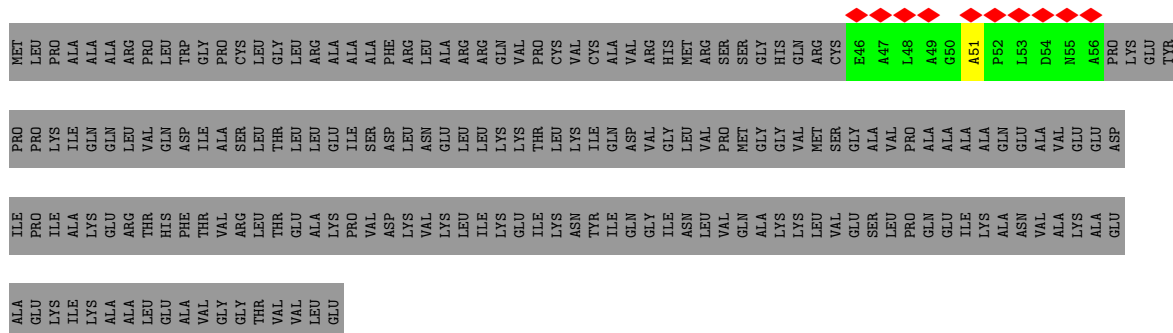
- Molecule 84: Large ribosomal subunit protein mL66



- Molecule 85: Large ribosomal subunit protein mL65



- Molecule 86: Large ribosomal subunit protein bL12m



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 114776                                  | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | TFS KRIOS                               | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 30                                      | Depositor |
| Minimum defocus (nm)                 | 800                                     | Depositor |
| Maximum defocus (nm)                 | 1600                                    | Depositor |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K3 (6k x 4k)                      | Depositor |
| Maximum map value                    | 0.321                                   | Depositor |
| Minimum map value                    | -0.071                                  | Depositor |
| Average map value                    | 0.003                                   | Depositor |
| Map value standard deviation         | 0.014                                   | Depositor |
| Recommended contour level            | 0.04                                    | Depositor |
| Map size ( $\text{\AA}$ )            | 424.96, 424.96, 424.96                  | wwPDB     |
| Map dimensions                       | 512, 512, 512                           | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 0.83, 0.83, 0.83                        | Depositor |



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, NAD, GDP, MG, PSU, B8T, K, SPD, FES, MA6, RSQ, 5MC, OMG, ZN, ATP, OMU, G34, ACE, 2MG, 5F0, 1MA

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

| Mol | Chain | Bond lengths |             | Bond angles |             |
|-----|-------|--------------|-------------|-------------|-------------|
|     |       | RMSZ         | # $ Z  > 5$ | RMSZ        | # $ Z  > 5$ |
| 1   | A     | 0.09         | 0/36048     | 0.21        | 0/56112     |
| 2   | B     | 0.08         | 0/1627      | 0.20        | 0/2527      |
| 3   | D     | 0.09         | 0/1896      | 0.24        | 0/2549      |
| 4   | E     | 0.08         | 0/2475      | 0.22        | 0/3355      |
| 5   | F     | 0.08         | 0/2090      | 0.23        | 0/2842      |
| 6   | H     | 0.07         | 0/837       | 0.19        | 0/1124      |
| 7   | I     | 0.08         | 0/1392      | 0.23        | 0/1880      |
| 8   | J     | 0.08         | 0/1348      | 0.19        | 0/1813      |
| 9   | K     | 0.09         | 0/1497      | 0.23        | 0/2031      |
| 10  | L     | 0.08         | 0/905       | 0.23        | 0/1218      |
| 11  | M     | 0.09         | 0/2368      | 0.24        | 0/3195      |
| 12  | N     | 0.09         | 0/1833      | 0.24        | 0/2468      |
| 13  | O     | 0.09         | 0/1283      | 0.22        | 0/1727      |
| 14  | P     | 0.09         | 0/1199      | 0.24        | 0/1623      |
| 15  | Q     | 0.09         | 0/2039      | 0.23        | 0/2750      |
| 16  | R     | 0.09         | 0/1175      | 0.19        | 0/1572      |
| 17  | S     | 0.09         | 0/1320      | 0.25        | 0/1789      |
| 18  | T     | 0.09         | 0/1403      | 0.23        | 0/1886      |
| 19  | U     | 0.11         | 0/1280      | 0.25        | 0/1732      |
| 20  | V     | 0.07         | 0/1721      | 0.22        | 0/2333      |
| 21  | W     | 0.08         | 0/926       | 0.21        | 0/1244      |
| 22  | X     | 0.08         | 0/2099      | 0.19        | 0/2837      |
| 23  | Y     | 0.08         | 0/1593      | 0.18        | 0/2136      |
| 24  | Z     | 0.08         | 0/1021      | 0.25        | 0/1378      |
| 25  | AA    | 0.08         | 0/22537     | 0.20        | 0/35085     |
| 26  | AB    | 0.07         | 0/1871      | 0.22        | 0/2531      |
| 27  | AC    | 0.07         | 0/1113      | 0.20        | 0/1505      |
| 28  | AD    | 0.07         | 0/2783      | 0.19        | 0/3724      |
| 29  | AE    | 0.07         | 0/989       | 0.19        | 0/1335      |
| 30  | AF    | 0.07         | 0/1767      | 0.19        | 0/2373      |
| 31  | AG    | 0.06         | 0/2616      | 0.18        | 0/3505      |

| Mol | Chain | Bond lengths |         | Bond angles |         |
|-----|-------|--------------|---------|-------------|---------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5 |
| 32  | AH    | 0.08         | 0/1178  | 0.23        | 0/1598  |
| 33  | AI    | 0.08         | 0/1030  | 0.23        | 0/1386  |
| 34  | AJ    | 0.07         | 0/855   | 0.21        | 0/1148  |
| 35  | AK    | 0.06         | 0/880   | 0.18        | 0/1182  |
| 36  | AL    | 0.06         | 0/1477  | 0.17        | 0/1974  |
| 37  | AM    | 0.06         | 0/963   | 0.19        | 0/1295  |
| 38  | AN    | 0.07         | 0/886   | 0.20        | 0/1199  |
| 39  | AO    | 0.06         | 0/1648  | 0.19        | 0/2243  |
| 40  | AP    | 0.07         | 0/798   | 0.18        | 0/1070  |
| 41  | AQ    | 0.12         | 0/754   | 0.20        | 0/1003  |
| 42  | AR    | 0.06         | 0/2456  | 0.18        | 0/3317  |
| 43  | AS    | 0.06         | 0/1138  | 0.18        | 0/1533  |
| 44  | AT    | 0.07         | 0/1402  | 0.20        | 0/1883  |
| 45  | AU    | 0.05         | 0/1510  | 0.16        | 0/2025  |
| 46  | AV    | 0.06         | 0/3030  | 0.17        | 0/4093  |
| 47  | AW    | 0.08         | 0/801   | 0.20        | 0/1079  |
| 48  | AX    | 0.06         | 0/2921  | 0.19        | 0/3954  |
| 49  | AY    | 0.07         | 0/1046  | 0.18        | 0/1410  |
| 50  | AZ    | 0.05         | 0/857   | 0.16        | 0/1141  |
| 51  | A0    | 0.07         | 0/1834  | 0.20        | 0/2484  |
| 52  | A1    | 0.06         | 0/2293  | 0.19        | 0/3102  |
| 53  | A2    | 0.12         | 0/947   | 0.22        | 0/1266  |
| 54  | A3    | 0.07         | 0/636   | 0.19        | 0/839   |
| 55  | A4    | 0.07         | 0/4427  | 0.19        | 0/5987  |
| 56  | Ax    | 0.08         | 0/1511  | 0.21        | 0/2341  |
| 57  | Az    | 0.06         | 0/185   | 0.16        | 0/285   |
| 58  | 0     | 0.08         | 0/913   | 0.18        | 0/1224  |
| 59  | 1     | 0.07         | 0/445   | 0.20        | 0/591   |
| 60  | 2     | 0.07         | 0/383   | 0.18        | 0/507   |
| 61  | 3     | 0.08         | 0/853   | 0.21        | 0/1136  |
| 62  | 4     | 0.07         | 0/350   | 0.18        | 0/461   |
| 63  | 5     | 0.09         | 0/3305  | 0.23        | 0/4502  |
| 64  | 6     | 0.07         | 0/3043  | 0.21        | 0/4140  |
| 65  | 7     | 0.08         | 0/2447  | 0.22        | 0/3310  |
| 66  | 8     | 0.08         | 0/1209  | 0.20        | 0/1628  |
| 67  | 9     | 0.07         | 0/1025  | 0.20        | 0/1379  |
| 68  | a     | 0.08         | 0/866   | 0.22        | 0/1174  |
| 69  | b     | 0.07         | 0/1219  | 0.23        | 0/1651  |
| 70  | c     | 0.08         | 0/2347  | 0.20        | 0/3171  |
| 71  | d     | 0.07         | 0/2039  | 0.21        | 0/2759  |
| 72  | e     | 0.07         | 0/1970  | 0.22        | 0/2658  |
| 73  | f     | 0.07         | 0/1273  | 0.21        | 0/1716  |
| 74  | g     | 0.08         | 0/1151  | 0.21        | 0/1569  |

| Mol | Chain | Bond lengths |          | Bond angles |          |
|-----|-------|--------------|----------|-------------|----------|
|     |       | RMSZ         | # Z  >5  | RMSZ        | # Z  >5  |
| 75  | h     | 0.07         | 0/918    | 0.18        | 0/1249   |
| 76  | i     | 0.08         | 0/850    | 0.20        | 0/1135   |
| 77  | j     | 0.08         | 0/760    | 0.18        | 0/1023   |
| 78  | k     | 0.07         | 0/749    | 0.18        | 0/1010   |
| 79  | l     | 0.06         | 0/707    | 0.19        | 0/960    |
| 80  | m     | 0.06         | 0/805    | 0.19        | 0/1081   |
| 81  | o     | 0.08         | 0/819    | 0.22        | 0/1097   |
| 82  | p     | 0.07         | 0/1197   | 0.18        | 0/1606   |
| 83  | q     | 0.09         | 0/1151   | 0.19        | 0/1556   |
| 84  | r     | 0.07         | 0/1362   | 0.20        | 0/1846   |
| 85  | s     | 0.09         | 0/3217   | 0.22        | 0/4369   |
| 86  | t     | 0.04         | 0/72     | 0.17        | 0/98     |
| All | All   | 0.08         | 0/179959 | 0.21        | 0/255622 |

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 |
|-----|-------|---------------------|---------------------|
| 14  | P     | 0                   | 1                   |
| 66  | 8     | 0                   | 1                   |
| All | All   | 0                   | 2                   |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 66  | 8     | 169 | PHE  | Peptide |
| 14  | P     | 72  | PHE  | 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   | A     | 32331 | 0        | 16416    | 412     | 0            |
| 2   | B     | 1524  | 0        | 779      | 21      | 0            |
| 3   | D     | 1859  | 0        | 1920     | 30      | 0            |
| 4   | E     | 2406  | 0        | 2415     | 27      | 0            |
| 5   | F     | 2031  | 0        | 2065     | 24      | 0            |
| 6   | H     | 823   | 0        | 873      | 12      | 0            |
| 7   | I     | 1362  | 0        | 1442     | 29      | 0            |
| 8   | J     | 1330  | 0        | 1407     | 23      | 0            |
| 9   | K     | 1455  | 0        | 1452     | 16      | 0            |
| 10  | L     | 890   | 0        | 941      | 18      | 0            |
| 11  | M     | 2314  | 0        | 2384     | 18      | 0            |
| 12  | N     | 1786  | 0        | 1817     | 19      | 0            |
| 13  | O     | 1259  | 0        | 1294     | 20      | 0            |
| 14  | P     | 1173  | 0        | 1165     | 16      | 0            |
| 15  | Q     | 1990  | 0        | 2031     | 28      | 0            |
| 16  | R     | 1154  | 0        | 1214     | 11      | 0            |
| 17  | S     | 1293  | 0        | 1365     | 16      | 0            |
| 18  | T     | 1369  | 0        | 1410     | 17      | 0            |
| 19  | U     | 1251  | 0        | 1232     | 20      | 0            |
| 20  | V     | 1676  | 0        | 1687     | 35      | 0            |
| 21  | W     | 904   | 0        | 935      | 9       | 0            |
| 22  | X     | 2044  | 0        | 2060     | 21      | 0            |
| 23  | Y     | 1556  | 0        | 1597     | 27      | 0            |
| 24  | Z     | 996   | 0        | 1044     | 15      | 0            |
| 25  | AA    | 20260 | 0        | 10285    | 269     | 0            |
| 26  | AB    | 1828  | 0        | 1815     | 18      | 0            |
| 27  | AC    | 1083  | 0        | 1088     | 14      | 0            |
| 28  | AD    | 2731  | 0        | 2804     | 35      | 0            |
| 29  | AE    | 972   | 0        | 1000     | 13      | 0            |
| 30  | AF    | 1725  | 0        | 1769     | 24      | 0            |
| 31  | AG    | 2561  | 0        | 2545     | 34      | 0            |
| 32  | AH    | 1152  | 0        | 1183     | 24      | 0            |
| 33  | AI    | 1020  | 0        | 1053     | 9       | 0            |
| 34  | AJ    | 839   | 0        | 887      | 11      | 0            |
| 35  | AK    | 862   | 0        | 885      | 18      | 0            |
| 36  | AL    | 1453  | 0        | 1540     | 12      | 0            |
| 37  | AM    | 942   | 0        | 965      | 14      | 0            |
| 38  | AN    | 868   | 0        | 928      | 11      | 0            |
| 39  | AO    | 1592  | 0        | 1557     | 19      | 0            |
| 40  | AP    | 781   | 0        | 806      | 7       | 0            |
| 41  | AQ    | 744   | 0        | 758      | 11      | 0            |
| 42  | AR    | 2409  | 0        | 2428     | 36      | 0            |
| 43  | AS    | 1111  | 0        | 1115     | 11      | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 44  | AT    | 1371  | 0        | 1393     | 12      | 0            |
| 45  | AU    | 1488  | 0        | 1499     | 11      | 0            |
| 46  | AV    | 2969  | 0        | 2961     | 45      | 0            |
| 47  | AW    | 789   | 0        | 802      | 11      | 0            |
| 48  | AX    | 2849  | 0        | 2844     | 54      | 0            |
| 49  | AY    | 1016  | 0        | 962      | 6       | 0            |
| 50  | AZ    | 839   | 0        | 858      | 16      | 0            |
| 51  | A0    | 1787  | 0        | 1796     | 32      | 0            |
| 52  | A1    | 2245  | 0        | 2276     | 27      | 0            |
| 53  | A2    | 935   | 0        | 971      | 10      | 0            |
| 54  | A3    | 625   | 0        | 699      | 5       | 0            |
| 55  | A4    | 4329  | 0        | 4350     | 59      | 0            |
| 56  | Ax    | 1378  | 0        | 703      | 26      | 0            |
| 57  | Az    | 167   | 0        | 83       | 1       | 0            |
| 58  | 0     | 898   | 0        | 916      | 14      | 0            |
| 59  | 1     | 440   | 0        | 480      | 5       | 0            |
| 60  | 2     | 377   | 0        | 406      | 4       | 0            |
| 61  | 3     | 832   | 0        | 883      | 13      | 0            |
| 62  | 4     | 342   | 0        | 361      | 7       | 0            |
| 63  | 5     | 3210  | 0        | 3206     | 45      | 0            |
| 64  | 6     | 2948  | 0        | 2841     | 42      | 0            |
| 65  | 7     | 2390  | 0        | 2397     | 40      | 0            |
| 66  | 8     | 1184  | 0        | 1210     | 18      | 0            |
| 67  | 9     | 997   | 0        | 987      | 17      | 0            |
| 68  | a     | 840   | 0        | 810      | 8       | 0            |
| 69  | b     | 1196  | 0        | 1195     | 16      | 0            |
| 70  | c     | 2299  | 0        | 2320     | 31      | 0            |
| 71  | d     | 1985  | 0        | 1976     | 25      | 0            |
| 72  | e     | 1931  | 0        | 1916     | 42      | 0            |
| 73  | f     | 1252  | 0        | 1269     | 22      | 0            |
| 74  | g     | 1113  | 0        | 1097     | 10      | 0            |
| 75  | h     | 895   | 0        | 881      | 2       | 0            |
| 76  | i     | 828   | 0        | 857      | 14      | 0            |
| 77  | j     | 745   | 0        | 746      | 10      | 0            |
| 78  | k     | 738   | 0        | 753      | 12      | 0            |
| 79  | l     | 688   | 0        | 674      | 14      | 0            |
| 80  | m     | 791   | 0        | 796      | 25      | 0            |
| 81  | o     | 798   | 0        | 804      | 17      | 0            |
| 82  | p     | 1179  | 0        | 1203     | 21      | 0            |
| 83  | q     | 1120  | 0        | 1099     | 12      | 0            |
| 84  | r     | 1322  | 0        | 1348     | 18      | 0            |
| 85  | s     | 3134  | 0        | 3121     | 39      | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 86  | t     | 72     | 0        | 67       | 1       | 0            |
| 87  | A     | 138    | 0        | 0        | 0       | 0            |
| 87  | A3    | 1      | 0        | 0        | 0       | 0            |
| 87  | AA    | 63     | 0        | 0        | 0       | 0            |
| 87  | AB    | 1      | 0        | 0        | 0       | 0            |
| 87  | AX    | 1      | 0        | 0        | 0       | 0            |
| 87  | D     | 2      | 0        | 0        | 0       | 0            |
| 87  | E     | 1      | 0        | 0        | 0       | 0            |
| 87  | g     | 1      | 0        | 0        | 0       | 0            |
| 88  | 6     | 1      | 0        | 0        | 0       | 0            |
| 88  | A     | 29     | 0        | 0        | 0       | 0            |
| 88  | AA    | 18     | 0        | 0        | 0       | 0            |
| 88  | D     | 1      | 0        | 0        | 0       | 0            |
| 88  | M     | 1      | 0        | 0        | 0       | 0            |
| 88  | W     | 1      | 0        | 0        | 0       | 0            |
| 88  | i     | 1      | 0        | 0        | 0       | 0            |
| 88  | o     | 1      | 0        | 0        | 0       | 0            |
| 89  | A     | 36     | 0        | 47       | 3       | 0            |
| 90  | B     | 7      | 0        | 8        | 2       | 0            |
| 91  | AA    | 44     | 0        | 26       | 1       | 0            |
| 92  | AA    | 10     | 0        | 19       | 0       | 0            |
| 93  | 0     | 1      | 0        | 0        | 0       | 0            |
| 93  | 4     | 1      | 0        | 0        | 0       | 0            |
| 93  | AO    | 1      | 0        | 0        | 0       | 0            |
| 94  | AP    | 4      | 0        | 0        | 0       | 0            |
| 94  | AT    | 4      | 0        | 0        | 0       | 0            |
| 94  | r     | 4      | 0        | 0        | 0       | 0            |
| 95  | AX    | 31     | 0        | 12       | 1       | 0            |
| 96  | AX    | 28     | 0        | 12       | 1       | 0            |
| All | All   | 171472 | 0        | 145296   | 1877    | 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 6.

All (1877) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1          | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-------------------|--------------------------|-------------------|
| 1:A:2485:U:H3   | 1:A:2650:C:N4     | 1.52                     | 1.06              |
| 1:A:2234:C:HO2' | 1:A:2688:C:HO2'   | 1.30                     | 0.80              |
| 64:6:179:VAL:O  | 64:6:183:ASP:HB2  | 1.82                     | 0.78              |
| 9:K:74:GLN:HE21 | 84:r:159:VAL:HG21 | 1.51                     | 0.76              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 82:p:84:SER:HB3   | 82:p:98:LYS:HB2   | 1.65                     | 0.76              |
| 25:AA:1021:U:OP2  | 53:A2:9:ARG:NH2   | 2.19                     | 0.74              |
| 25:AA:1053:A:N1   | 25:AA:1100:C:O2'  | 2.22                     | 0.72              |
| 65:7:163:MET:H    | 65:7:186:ASP:HB2  | 1.54                     | 0.72              |
| 2:B:44:A:H62      | 14:P:120:ARG:HH12 | 1.38                     | 0.72              |
| 25:AA:1562:G:H1'  | 25:AA:1583:MA6:H2 | 1.70                     | 0.72              |
| 8:J:20:ILE:HD11   | 8:J:42:ARG:HD3    | 1.72                     | 0.72              |
| 1:A:1777:A:N6     | 1:A:1780:U:OP2    | 2.23                     | 0.72              |
| 7:I:47:LEU:HD22   | 12:N:226:ILE:HG12 | 1.71                     | 0.72              |
| 25:AA:1422:G:H21  | 56:Ax:41:C:H1'    | 1.54                     | 0.71              |
| 1:A:1884:G:H1'    | 1:A:1895:C:H1'    | 1.70                     | 0.71              |
| 1:A:2139:U:H5''   | 24:Z:74:SER:HB2   | 1.72                     | 0.71              |
| 12:N:124:VAL:HG12 | 12:N:158:ARG:HE   | 1.53                     | 0.71              |
| 30:AF:52:ARG:HH22 | 31:AG:320:VAL:HA  | 1.54                     | 0.71              |
| 70:c:259:ARG:HB2  | 70:c:271:PHE:HB2  | 1.72                     | 0.71              |
| 56:Ax:5:A:H2      | 56:Ax:68:G:H22    | 1.36                     | 0.71              |
| 65:7:247:ASN:HD22 | 65:7:251:ILE:H    | 1.39                     | 0.70              |
| 1:A:2499:U:OP2    | 1:A:2504:A:N6     | 2.21                     | 0.70              |
| 1:A:2137:C:H5''   | 7:I:43:GLN:HE21   | 1.58                     | 0.69              |
| 9:K:178:LEU:HD11  | 84:r:94:ARG:HA    | 1.75                     | 0.69              |
| 22:X:7:PRO:HD2    | 22:X:10:LEU:HD12  | 1.73                     | 0.69              |
| 1:A:2259:C:O2'    | 1:A:2261:C:OP2    | 2.09                     | 0.69              |
| 48:AX:319:PRO:HG2 | 48:AX:322:ALA:HB2 | 1.75                     | 0.68              |
| 11:M:44:ARG:HG3   | 11:M:45:ARG:HG3   | 1.73                     | 0.68              |
| 25:AA:1557:A:H5'' | 34:AJ:72:LYS:HG3  | 1.75                     | 0.68              |
| 1:A:1763:A:N7     | 83:q:38:ARG:NH1   | 2.42                     | 0.68              |
| 65:7:112:PRO:HB2  | 65:7:267:PRO:HG2  | 1.74                     | 0.68              |
| 10:L:68:LYS:NZ    | 10:L:91:MET:SD    | 2.67                     | 0.68              |
| 63:5:204:VAL:HG11 | 63:5:279:PHE:HZ   | 1.58                     | 0.68              |
| 1:A:1805:A:OP2    | 20:V:94:HIS:NE2   | 2.25                     | 0.67              |
| 51:A0:28:PRO:HG3  | 51:A0:215:GLY:HA2 | 1.76                     | 0.67              |
| 85:s:177:LEU:HD23 | 85:s:238:ASN:HD22 | 1.58                     | 0.67              |
| 48:AX:80:PRO:HG2  | 48:AX:81:HIS:HD2  | 1.59                     | 0.67              |
| 1:A:2603:C:H4'    | 1:A:3090:G:H1'    | 1.76                     | 0.67              |
| 36:AL:180:LYS:HD2 | 36:AL:183:TRP:HE1 | 1.60                     | 0.67              |
| 64:6:367:ASP:OD1  | 64:6:370:ARG:NH1  | 2.28                     | 0.67              |
| 31:AG:90:ASN:HD21 | 52:A1:64:GLN:H    | 1.43                     | 0.67              |
| 1:A:2545:U:H5''   | 1:A:2546:G:H5'    | 1.75                     | 0.67              |
| 25:AA:773:U:H2'   | 25:AA:774:G:H8    | 1.60                     | 0.67              |
| 25:AA:1355:G:N2   | 25:AA:1356:A:N7   | 2.41                     | 0.67              |
| 2:B:26:A:N6       | 14:P:87:GLN:OE1   | 2.27                     | 0.66              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 20:V:31:ASP:O      | 20:V:34:LYS:O     | 2.12                     | 0.66              |
| 25:AA:929:A:H4'    | 28:AD:420:SER:HA  | 1.76                     | 0.66              |
| 1:A:1763:A:H5''    | 83:q:34:ARG:HH21  | 1.59                     | 0.66              |
| 25:AA:1294:A:OP1   | 26:AB:201:ASN:ND2 | 2.28                     | 0.66              |
| 6:H:99:THR:O       | 6:H:108:ARG:NH1   | 2.29                     | 0.66              |
| 1:A:2108:G:N7      | 12:N:67:LYS:NZ    | 2.43                     | 0.66              |
| 17:S:175:ARG:HB2   | 17:S:180:PHE:HB3  | 1.78                     | 0.66              |
| 68:a:41:ASP:HB3    | 68:a:46:ASN:HD22  | 1.59                     | 0.66              |
| 24:Z:78:ARG:O      | 24:Z:83:LYS:NZ    | 2.29                     | 0.66              |
| 72:e:110:ASP:HB3   | 72:e:113:ASP:HB2  | 1.78                     | 0.66              |
| 82:p:111:ILE:O     | 82:p:116:ARG:NH1  | 2.28                     | 0.66              |
| 1:A:2192:A:OP2     | 79:l:119:ARG:NH1  | 2.28                     | 0.65              |
| 25:AA:821:U:H2'    | 25:AA:822:G:H8    | 1.61                     | 0.65              |
| 20:V:31:ASP:OD1    | 20:V:35:ASN:ND2   | 2.29                     | 0.65              |
| 1:A:1689:C:O2      | 23:Y:213:ARG:NH2  | 2.29                     | 0.65              |
| 17:S:164:THR:HG23  | 69:b:107:GLN:HG2  | 1.79                     | 0.65              |
| 9:K:178:LEU:HD13   | 84:r:100:LEU:HD21 | 1.78                     | 0.65              |
| 22:X:163:ARG:HE    | 63:5:55:LEU:HD11  | 1.62                     | 0.65              |
| 28:AD:103:LEU:HD11 | 28:AD:123:ARG:HB2 | 1.77                     | 0.65              |
| 3:D:176:ALA:HB1    | 3:D:244:VAL:HG11  | 1.78                     | 0.65              |
| 74:g:84:TYR:OH     | 74:g:164:LYS:NZ   | 2.30                     | 0.65              |
| 1:A:2067:C:H4'     | 73:f:60:LYS:HD2   | 1.79                     | 0.65              |
| 56:Ax:9:C:O2'      | 56:Ax:10:A:N7     | 2.27                     | 0.65              |
| 1:A:2677:A:H2'     | 1:A:2678:A:C8     | 2.32                     | 0.65              |
| 26:AB:239:ASN:OD1  | 47:AW:119:LYS:NZ  | 2.30                     | 0.64              |
| 64:6:252:CYS:SG    | 64:6:296:ARG:NH1  | 2.70                     | 0.64              |
| 72:e:101:LYS:HZ1   | 72:e:107:ASP:HB3  | 1.62                     | 0.64              |
| 19:U:129:MET:HG3   | 71:d:82:ALA:HB2   | 1.79                     | 0.64              |
| 50:AZ:66:ARG:NH2   | 50:AZ:77:ASP:OD1  | 2.29                     | 0.64              |
| 1:A:2082:G:N2      | 24:Z:88:MET:SD    | 2.71                     | 0.64              |
| 1:A:1800:G:N1      | 1:A:1803:A:OP2    | 2.30                     | 0.64              |
| 4:E:69:ASP:OD1     | 4:E:154:ARG:NH1   | 2.31                     | 0.64              |
| 46:AV:177:SER:HB2  | 46:AV:367:CYS:HB3 | 1.80                     | 0.64              |
| 72:e:178:TRP:NE1   | 72:e:182:GLU:O    | 2.30                     | 0.64              |
| 16:R:122:ARG:NH1   | 17:S:72:GLU:OE2   | 2.30                     | 0.64              |
| 29:AE:26:ILE:HG23  | 29:AE:36:VAL:HG21 | 1.78                     | 0.64              |
| 30:AF:44:PRO:HD3   | 30:AF:75:LYS:HB2  | 1.80                     | 0.64              |
| 25:AA:942:A:N6     | 25:AA:1047:A:OP2  | 2.30                     | 0.64              |
| 30:AF:172:VAL:HG12 | 30:AF:240:ARG:HD3 | 1.80                     | 0.64              |
| 85:s:174:LEU:HD11  | 85:s:203:ARG:HD3  | 1.79                     | 0.64              |
| 19:U:11:ARG:NH2    | 20:V:212:LYS:O    | 2.31                     | 0.63              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 20:V:93:THR:HG22   | 20:V:112:GLU:HG3   | 1.79                     | 0.63              |
| 20:V:133:ILE:HD13  | 20:V:145:ARG:HD2   | 1.81                     | 0.63              |
| 71:d:98:SER:OG     | 71:d:215:ARG:NH2   | 2.32                     | 0.63              |
| 1:A:2972:A:H5''    | 12:N:184:PRO:HA    | 1.80                     | 0.63              |
| 65:7:159:LYS:NZ    | 68:a:92:LEU:O      | 2.31                     | 0.63              |
| 1:A:2409:A:O2'     | 63:5:270:ILE:O     | 2.17                     | 0.63              |
| 18:T:69:HIS:HD2    | 18:T:114:VAL:HG13  | 1.64                     | 0.63              |
| 63:5:150:GLN:HE22  | 63:5:412:ARG:HG3   | 1.64                     | 0.63              |
| 20:V:31:ASP:O      | 20:V:34:LYS:C      | 2.42                     | 0.63              |
| 55:A4:263:ILE:HG23 | 55:A4:275:ALA:HB1  | 1.81                     | 0.63              |
| 29:AE:35:ILE:HD13  | 36:AL:88:VAL:HG13  | 1.81                     | 0.62              |
| 65:7:148:MET:HE2   | 65:7:257:ILE:HG12  | 1.79                     | 0.62              |
| 15:Q:96:ARG:HH22   | 15:Q:285:GLU:HB3   | 1.64                     | 0.62              |
| 25:AA:1046:A:O4'   | 91:AA:1701:NAD:N6A | 2.32                     | 0.62              |
| 31:AG:209:LEU:HD12 | 31:AG:213:LEU:HD11 | 1.82                     | 0.62              |
| 7:I:167:ILE:O      | 7:I:170:THR:OG1    | 2.17                     | 0.62              |
| 25:AA:1402:A:OP1   | 35:AK:51:ARG:NH2   | 2.30                     | 0.62              |
| 55:A4:573:ALA:HB2  | 55:A4:604:LYS:HD2  | 1.82                     | 0.62              |
| 85:s:63:ILE:HA     | 85:s:66:TRP:CD1    | 2.34                     | 0.62              |
| 1:A:1886:G:H1      | 76:i:61:GLY:HA3    | 1.64                     | 0.62              |
| 85:s:152:GLN:HA    | 85:s:156:TYR:HB2   | 1.81                     | 0.62              |
| 1:A:3211:C:H4'     | 1:A:3212:C:H5      | 1.64                     | 0.62              |
| 25:AA:1529:A:H1'   | 46:AV:66:PRO:HD3   | 1.80                     | 0.62              |
| 1:A:1672:C:O2'     | 18:T:143:ARG:O     | 2.16                     | 0.62              |
| 1:A:1745:U:O4      | 61:3:108:LYS:NZ    | 2.33                     | 0.62              |
| 42:AR:162:SER:O    | 42:AR:170:ARG:NH1  | 2.31                     | 0.62              |
| 48:AX:181:PRO:HB2  | 48:AX:233:VAL:HG12 | 1.81                     | 0.62              |
| 5:F:55:VAL:HG21    | 5:F:61:PRO:HG3     | 1.82                     | 0.62              |
| 25:AA:702:C:O2'    | 25:AA:842:C:O2     | 2.17                     | 0.62              |
| 30:AF:50:TYR:O     | 30:AF:66:ARG:NH2   | 2.27                     | 0.62              |
| 72:e:188:ALA:O     | 72:e:191:THR:OG1   | 2.15                     | 0.62              |
| 25:AA:1199:G:N1    | 25:AA:1422:G:OP2   | 2.32                     | 0.62              |
| 1:A:2103:A:HO2'    | 24:Z:35:LYS:N      | 1.98                     | 0.62              |
| 7:I:128:ASN:ND2    | 7:I:147:PHE:O      | 2.33                     | 0.62              |
| 30:AF:126:TYR:O    | 30:AF:134:GLN:NE2  | 2.33                     | 0.62              |
| 84:r:71:PRO:HD2    | 84:r:107:LEU:HD23  | 1.81                     | 0.62              |
| 1:A:1884:G:N3      | 1:A:1895:C:O2'     | 2.32                     | 0.61              |
| 25:AA:704:U:H5''   | 51:A0:53:ARG:HB2   | 1.81                     | 0.61              |
| 28:AD:307:LYS:NZ   | 42:AR:103:TYR:OH   | 2.32                     | 0.61              |
| 1:A:2458:A:O2'     | 4:E:215:PHE:O      | 2.18                     | 0.61              |
| 25:AA:949:U:O2'    | 38:AN:29:ARG:NH1   | 2.33                     | 0.61              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:N:124:VAL:HA    | 12:N:158:ARG:HH21  | 1.65                     | 0.61              |
| 37:AM:64:LYS:HE3   | 42:AR:154:THR:HB   | 1.82                     | 0.61              |
| 3:D:195:ASN:H      | 3:D:207:ILE:HB     | 1.66                     | 0.61              |
| 33:AI:153:GLY:O    | 33:AI:158:ARG:NH1  | 2.33                     | 0.61              |
| 4:E:78:CYS:HB3     | 4:E:81:LYS:HB2     | 1.83                     | 0.61              |
| 41:AQ:49:CYS:SG    | 41:AQ:50:ARG:NH1   | 2.74                     | 0.61              |
| 72:e:255:VAL:HB    | 72:e:259:GLU:HG3   | 1.83                     | 0.61              |
| 17:S:127:ARG:NH2   | 17:S:157:GLU:OE1   | 2.34                     | 0.61              |
| 1:A:2537:G:O2'     | 1:A:2634:U:OP2     | 2.18                     | 0.61              |
| 25:AA:1470:A:H2'   | 25:AA:1471:A:H8    | 1.66                     | 0.61              |
| 31:AG:389:ARG:NH1  | 31:AG:390:LYS:O    | 2.34                     | 0.61              |
| 48:AX:125:LEU:HD11 | 48:AX:310:LEU:HG   | 1.82                     | 0.61              |
| 52:A1:214:LEU:O    | 52:A1:218:ASN:ND2  | 2.34                     | 0.61              |
| 1:A:3150:U:H2'     | 1:A:3151:A:H8      | 1.65                     | 0.61              |
| 5:F:272:LYS:NZ     | 76:i:65:ASN:OD1    | 2.33                     | 0.60              |
| 8:J:114:LEU:HD21   | 79:l:101:LEU:HD21  | 1.83                     | 0.60              |
| 1:A:2055:U:H2'     | 1:A:2056:G:H8      | 1.65                     | 0.60              |
| 48:AX:161:TRP:O    | 48:AX:180:GLN:NE2  | 2.34                     | 0.60              |
| 48:AX:206:GLU:HG3  | 48:AX:249:ARG:HH12 | 1.66                     | 0.60              |
| 78:k:10:LEU:O      | 78:k:46:ASN:ND2    | 2.34                     | 0.60              |
| 25:AA:1239:C:H2'   | 25:AA:1240:A:H8    | 1.66                     | 0.60              |
| 11:M:30:ASN:OD1    | 81:o:86:ARG:NH2    | 2.34                     | 0.60              |
| 24:Z:99:VAL:HG11   | 77:j:77:VAL:HG22   | 1.82                     | 0.60              |
| 25:AA:893:G:H4'    | 34:AJ:98:GLU:HG2   | 1.84                     | 0.60              |
| 25:AA:952:A:N3     | 25:AA:954:C:N4     | 2.49                     | 0.60              |
| 71:d:211:GLN:HA    | 71:d:248:PHE:O     | 2.01                     | 0.60              |
| 1:A:3068:G:OP2     | 1:A:3068:G:N2      | 2.30                     | 0.60              |
| 5:F:224:GLU:OE2    | 83:q:32:ARG:NH2    | 2.35                     | 0.60              |
| 21:W:125:VAL:HG21  | 64:6:64:GLU:HG2    | 1.83                     | 0.60              |
| 25:AA:1412:G:OP1   | 48:AX:279:LYS:NZ   | 2.34                     | 0.60              |
| 9:K:143:GLU:OE1    | 69:b:136:LYS:NZ    | 2.34                     | 0.60              |
| 20:V:79:VAL:HG12   | 20:V:86:VAL:HG12   | 1.82                     | 0.60              |
| 1:A:1689:C:OP2     | 22:X:5:LYS:NZ      | 2.27                     | 0.60              |
| 1:A:2909:G:OP1     | 59:1:63:ARG:NH1    | 2.34                     | 0.60              |
| 46:AV:167:VAL:HG13 | 46:AV:172:ALA:HB3  | 1.83                     | 0.60              |
| 1:A:1857:U:H2'     | 1:A:1858:G:C8      | 2.37                     | 0.60              |
| 1:A:2197:G:H4'     | 79:l:127:TRP:HE1   | 1.67                     | 0.60              |
| 25:AA:949:U:O2'    | 38:AN:46:ARG:NH1   | 2.35                     | 0.60              |
| 82:p:94:LYS:HE2    | 82:p:96:ASN:HB2    | 1.83                     | 0.60              |
| 1:A:2531:U:O4      | 3:D:246:ARG:NH2    | 2.35                     | 0.59              |
| 25:AA:1530:A:OP1   | 51:A0:29:ARG:NH2   | 2.35                     | 0.59              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 15:Q:183:LEU:HD21  | 15:Q:219:GLU:HG2   | 1.84                     | 0.59              |
| 25:AA:1515:G:H2'   | 25:AA:1516:G:H8    | 1.68                     | 0.59              |
| 32:AH:92:GLU:OE1   | 32:AH:141:ARG:NH1  | 2.35                     | 0.59              |
| 55:A4:443:ASP:HB3  | 55:A4:446:LYS:HE2  | 1.84                     | 0.59              |
| 85:s:111:LYS:NZ    | 85:s:384:ASP:OD1   | 2.36                     | 0.59              |
| 20:V:129:LYS:HB2   | 20:V:149:ARG:HH12  | 1.68                     | 0.59              |
| 25:AA:947:U:OP1    | 36:AL:162:GLN:NE2  | 2.34                     | 0.59              |
| 1:A:2416:U:OP2     | 85:s:165:ARG:NH1   | 2.35                     | 0.59              |
| 25:AA:744:A:OP1    | 37:AM:46:ARG:NH2   | 2.36                     | 0.59              |
| 63:5:113:LEU:HD12  | 63:5:311:ALA:HB1   | 1.84                     | 0.59              |
| 66:8:91:PRO:HB2    | 66:8:93:LYS:HG2    | 1.84                     | 0.59              |
| 1:A:2182:G:N3      | 1:A:2199:A:O2'     | 2.33                     | 0.59              |
| 1:A:2854:U:H4'     | 61:3:138:PRO:HG2   | 1.83                     | 0.59              |
| 14:P:94:VAL:HB     | 14:P:103:VAL:HG23  | 1.84                     | 0.59              |
| 65:7:83:LYS:NZ     | 65:7:120:THR:O     | 2.35                     | 0.59              |
| 8:J:88:SER:HA      | 8:J:151:LEU:HD11   | 1.84                     | 0.59              |
| 20:V:80:ILE:HB     | 20:V:85:TRP:HB2    | 1.84                     | 0.59              |
| 55:A4:343:ARG:HA   | 55:A4:378:LEU:HD13 | 1.84                     | 0.59              |
| 24:Z:117:ILE:O     | 81:o:45:ASN:ND2    | 2.35                     | 0.59              |
| 34:AJ:62:VAL:HA    | 34:AJ:83:VAL:HG12  | 1.85                     | 0.59              |
| 48:AX:268:LEU:HD21 | 48:AX:293:LEU:HD23 | 1.84                     | 0.59              |
| 52:A1:187:LYS:HE3  | 52:A1:191:ILE:HD11 | 1.84                     | 0.59              |
| 1:A:2277:U:H2'     | 1:A:2278:A:H8      | 1.67                     | 0.59              |
| 55:A4:556:LYS:NZ   | 55:A4:560:GLU:OE2  | 2.36                     | 0.59              |
| 50:AZ:54:ASN:ND2   | 50:AZ:57:THR:OG1   | 2.35                     | 0.59              |
| 64:6:90:ILE:HA     | 77:j:112:LYS:HB2   | 1.82                     | 0.59              |
| 66:8:99:ARG:HG2    | 72:e:89:LEU:HD11   | 1.84                     | 0.59              |
| 55:A4:267:VAL:HG21 | 55:A4:296:ALA:HB1  | 1.85                     | 0.59              |
| 68:a:75:ILE:HD13   | 70:c:255:SER:HB2   | 1.84                     | 0.58              |
| 1:A:1871:A:N7      | 1:A:1902:C:N4      | 2.51                     | 0.58              |
| 25:AA:1440:G:H2'   | 25:AA:1441:A:C8    | 2.38                     | 0.58              |
| 26:AB:156:GLU:OE1  | 31:AG:163:HIS:ND1  | 2.35                     | 0.58              |
| 63:5:307:ASP:OD1   | 63:5:310:ARG:NH2   | 2.35                     | 0.58              |
| 70:c:42:GLN:NE2    | 76:i:36:LEU:O      | 2.35                     | 0.58              |
| 79:l:76:ASN:ND2    | 79:l:83:ASP:OD1    | 2.37                     | 0.58              |
| 8:J:28:LEU:HD13    | 79:l:56:LEU:HD22   | 1.84                     | 0.58              |
| 15:Q:121:THR:HG22  | 15:Q:171:VAL:HA    | 1.85                     | 0.58              |
| 25:AA:1132:U:H2'   | 25:AA:1133:C:H6    | 1.67                     | 0.58              |
| 25:AA:1154:A:OP2   | 54:A3:155:ARG:NH2  | 2.37                     | 0.58              |
| 28:AD:283:GLU:O    | 28:AD:356:GLN:NE2  | 2.37                     | 0.58              |
| 39:AO:225:GLN:HE21 | 45:AU:47:ALA:HB3   | 1.67                     | 0.58              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 68:a:77:ARG:NH2    | 70:c:293:GLU:OE1   | 2.33                     | 0.58              |
| 1:A:1897:A:H2'     | 1:A:1898:A:H8      | 1.68                     | 0.58              |
| 1:A:1905:C:OP1     | 5:F:117:ARG:NH1    | 2.35                     | 0.58              |
| 1:A:2945:A:O2'     | 1:A:2947:U:O4      | 2.21                     | 0.58              |
| 25:AA:1398:U:H2'   | 25:AA:1399:A:H8    | 1.69                     | 0.58              |
| 30:AF:122:GLN:NE2  | 30:AF:138:GLU:O    | 2.35                     | 0.58              |
| 45:AU:77:GLU:HG2   | 45:AU:80:ARG:HH22  | 1.68                     | 0.58              |
| 69:b:15:LEU:HD22   | 70:c:222:GLN:HE22  | 1.68                     | 0.58              |
| 46:AV:236:LEU:HD21 | 46:AV:323:GLU:HB2  | 1.85                     | 0.58              |
| 1:A:2095:U:OP2     | 11:M:57:ARG:NH1    | 2.33                     | 0.58              |
| 5:F:253:MET:HE3    | 5:F:259:LEU:HD22   | 1.85                     | 0.58              |
| 25:AA:841:A:OP1    | 37:AM:39:ASN:ND2   | 2.35                     | 0.58              |
| 38:AN:8:VAL:O      | 38:AN:11:ARG:NH1   | 2.37                     | 0.58              |
| 43:AS:111:GLU:HB2  | 43:AS:117:LEU:HD13 | 1.85                     | 0.58              |
| 48:AX:260:VAL:HB   | 48:AX:306:ILE:HG23 | 1.84                     | 0.58              |
| 63:5:166:THR:O     | 85:s:287:LYS:NZ    | 2.33                     | 0.58              |
| 65:7:220:GLU:HG2   | 65:7:253:LYS:HG2   | 1.85                     | 0.58              |
| 85:s:242:ARG:NH1   | 85:s:292:CYS:O     | 2.36                     | 0.58              |
| 25:AA:674:U:H2'    | 25:AA:675:A:H8     | 1.68                     | 0.58              |
| 25:AA:1287:A:OP2   | 28:AD:260:LYS:NZ   | 2.33                     | 0.58              |
| 42:AR:194:GLN:HE22 | 42:AR:199:LYS:H    | 1.51                     | 0.58              |
| 63:5:115:GLU:HB2   | 63:5:119:GLN:HB2   | 1.86                     | 0.58              |
| 77:j:100:GLU:HG2   | 77:j:104:LYS:HE3   | 1.85                     | 0.58              |
| 64:6:255:LEU:HD12  | 64:6:256:PRO:HD2   | 1.85                     | 0.58              |
| 72:e:164:LYS:HE2   | 72:e:167:ASP:HA    | 1.85                     | 0.58              |
| 1:A:2737:U:O2'     | 1:A:3084:A:N3      | 2.37                     | 0.58              |
| 1:A:2408:U:H2'     | 1:A:2409:A:H8      | 1.69                     | 0.58              |
| 1:A:3188:U:OP2     | 62:4:84:ARG:NE     | 2.36                     | 0.58              |
| 25:AA:1440:G:H2'   | 25:AA:1441:A:H8    | 1.69                     | 0.58              |
| 30:AF:119:LYS:NZ   | 48:AX:398:LEU:O    | 2.36                     | 0.58              |
| 64:6:214:TRP:HB3   | 64:6:272:LEU:HD11  | 1.86                     | 0.58              |
| 65:7:51:GLU:OE2    | 65:7:54:ARG:NH1    | 2.37                     | 0.58              |
| 78:k:42:VAL:O      | 78:k:45:THR:OG1    | 2.20                     | 0.58              |
| 1:A:1697:A:N3      | 1:A:1703:C:O2'     | 2.37                     | 0.57              |
| 7:I:122:LEU:HB3    | 7:I:124:LYS:HE2    | 1.86                     | 0.57              |
| 26:AB:243:PRO:O    | 26:AB:247:HIS:ND1  | 2.31                     | 0.57              |
| 61:3:179:LYS:O     | 64:6:370:ARG:NH2   | 2.37                     | 0.57              |
| 25:AA:1132:U:H2'   | 25:AA:1133:C:C6    | 2.39                     | 0.57              |
| 25:AA:1455:U:OP1   | 31:AG:278:THR:OG1  | 2.22                     | 0.57              |
| 31:AG:126:LYS:H    | 31:AG:131:ILE:HD11 | 1.69                     | 0.57              |
| 1:A:2519:G:N7      | 3:D:230:SER:OG     | 2.35                     | 0.57              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:AA:897:C:OP2    | 34:AJ:116:GLN:NE2  | 2.36                     | 0.57              |
| 25:AA:1587:U:H2'   | 25:AA:1588:G:H8    | 1.68                     | 0.57              |
| 31:AG:273:GLU:HG2  | 31:AG:282:GLU:HG2  | 1.86                     | 0.57              |
| 48:AX:108:LEU:HD23 | 48:AX:141:VAL:HG21 | 1.86                     | 0.57              |
| 48:AX:214:GLU:OE1  | 48:AX:228:GLN:NE2  | 2.37                     | 0.57              |
| 3:D:173:ALA:HB1    | 3:D:188:PRO:HG3    | 1.87                     | 0.57              |
| 14:P:94:VAL:HG23   | 14:P:132:LEU:HD21  | 1.85                     | 0.57              |
| 20:V:135:TRP:HB3   | 20:V:143:ARG:HD2   | 1.85                     | 0.57              |
| 19:U:21:ARG:NH1    | 23:Y:143:ASP:OD1   | 2.34                     | 0.57              |
| 20:V:123:VAL:HA    | 20:V:130:PRO:HA    | 1.85                     | 0.57              |
| 25:AA:808:C:OP1    | 51:A0:19:ARG:NH1   | 2.37                     | 0.57              |
| 65:7:284:HIS:HB3   | 65:7:323:MET:HE2   | 1.87                     | 0.57              |
| 1:A:1871:A:N3      | 61:3:104:ARG:NH2   | 2.52                     | 0.57              |
| 1:A:1990:G:OP1     | 3:D:269:ARG:NH2    | 2.37                     | 0.57              |
| 1:A:2325:U:O2'     | 13:O:82:GLU:OE2    | 2.21                     | 0.57              |
| 16:R:96:GLU:O      | 17:S:105:GLN:NE2   | 2.32                     | 0.57              |
| 28:AD:244:LEU:HD22 | 28:AD:343:LEU:HD23 | 1.86                     | 0.57              |
| 50:AZ:86:LYS:HG2   | 50:AZ:89:ARG:HH22  | 1.67                     | 0.57              |
| 65:7:114:ASP:HB2   | 65:7:117:LYS:HB2   | 1.86                     | 0.57              |
| 85:s:246:GLN:NE2   | 85:s:354:PRO:O     | 2.38                     | 0.57              |
| 1:A:2395:A:O2'     | 63:5:384:GLN:NE2   | 2.38                     | 0.57              |
| 2:B:43:G:H2'       | 2:B:44:A:C8        | 2.39                     | 0.57              |
| 19:U:133:GLU:OE2   | 19:U:137:ARG:NH2   | 2.37                     | 0.57              |
| 22:X:238:LEU:HD11  | 67:9:101:GLU:HG2   | 1.86                     | 0.57              |
| 43:AS:78:TYR:HA    | 43:AS:134:ARG:HA   | 1.87                     | 0.57              |
| 1:A:2191:A:H4'     | 8:J:142:ARG:HG2    | 1.87                     | 0.57              |
| 56:Ax:69:U:H2'     | 56:Ax:70:A:H8      | 1.70                     | 0.57              |
| 1:A:3127:G:N2      | 1:A:3130:A:OP2     | 2.38                     | 0.57              |
| 15:Q:96:ARG:NH1    | 15:Q:285:GLU:OE1   | 2.38                     | 0.57              |
| 56:Ax:67:C:H2'     | 56:Ax:68:G:C8      | 2.40                     | 0.57              |
| 74:g:110:ILE:HD11  | 74:g:157:LEU:HD13  | 1.86                     | 0.57              |
| 1:A:1672:C:OP1     | 18:T:44:LYS:N      | 2.36                     | 0.56              |
| 1:A:1746:A:OP2     | 22:X:55:LYS:NZ     | 2.35                     | 0.56              |
| 1:A:2410:U:HO2'    | 63:5:96:HIS:HD1    | 1.53                     | 0.56              |
| 4:E:50:ASP:O       | 13:O:138:ARG:NH2   | 2.37                     | 0.56              |
| 1:A:1799:U:O4      | 20:V:34:LYS:NZ     | 2.38                     | 0.56              |
| 1:A:2822:C:O2'     | 1:A:2915:C:OP2     | 2.23                     | 0.56              |
| 7:I:103:ALA:HB3    | 78:k:39:SER:HA     | 1.86                     | 0.56              |
| 7:I:147:PHE:HE1    | 7:I:153:LEU:HD21   | 1.70                     | 0.56              |
| 9:K:174:GLU:HG2    | 84:r:56:THR:HG21   | 1.87                     | 0.56              |
| 42:AR:323:GLU:H    | 42:AR:326:ASN:HB2  | 1.70                     | 0.56              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 67:9:113:ASN:HB3   | 67:9:116:LYS:HB3   | 1.87                     | 0.56              |
| 74:g:73:GLN:HB3    | 74:g:162:LEU:HD11  | 1.85                     | 0.56              |
| 1:A:2421:G:H5''    | 67:9:24:LYS:HG2    | 1.88                     | 0.56              |
| 18:T:127:ASN:O     | 71:d:230:ARG:NH2   | 2.38                     | 0.56              |
| 33:AI:112:CYS:HB2  | 33:AI:122:LYS:HG3  | 1.86                     | 0.56              |
| 34:AJ:109:LEU:HD22 | 34:AJ:129:LYS:HG2  | 1.86                     | 0.56              |
| 35:AK:60:ASN:O     | 35:AK:68:GLN:NE2   | 2.38                     | 0.56              |
| 38:AN:83:GLU:OE1   | 44:AT:85:GLN:NE2   | 2.38                     | 0.56              |
| 44:AT:42:GLU:OE1   | 44:AT:45:ARG:NH2   | 2.36                     | 0.56              |
| 46:AV:317:LEU:HB2  | 46:AV:320:GLU:HG3  | 1.88                     | 0.56              |
| 48:AX:210:TRP:NE1  | 48:AX:216:THR:OG1  | 2.33                     | 0.56              |
| 59:1:13:SER:HB3    | 59:1:36:ARG:HH21   | 1.69                     | 0.56              |
| 62:4:87:ARG:NH2    | 62:4:102:GLN:O     | 2.35                     | 0.56              |
| 72:e:213:TYR:HD1   | 72:e:271:GLN:HG3   | 1.71                     | 0.56              |
| 85:s:145:VAL:HG21  | 85:s:187:LEU:HD11  | 1.88                     | 0.56              |
| 1:A:2256:U:O2'     | 17:S:118:ASN:ND2   | 2.38                     | 0.56              |
| 1:A:2273:A:O2'     | 16:R:16:ASP:OD2    | 2.22                     | 0.56              |
| 3:D:257:ILE:HG23   | 3:D:262:ARG:HB3    | 1.87                     | 0.56              |
| 36:AL:95:LEU:HD11  | 36:AL:106:ILE:HD12 | 1.87                     | 0.56              |
| 44:AT:93:LYS:HE3   | 45:AU:116:LEU:HD11 | 1.87                     | 0.56              |
| 1:A:2361:G:H3'     | 1:A:2362:A:H8      | 1.70                     | 0.56              |
| 3:D:201:GLY:O      | 63:5:30:ALA:N      | 2.39                     | 0.56              |
| 64:6:222:ASP:O     | 64:6:266:HIS:ND1   | 2.39                     | 0.56              |
| 1:A:2871:U:OP2     | 61:3:143:ARG:NH2   | 2.38                     | 0.56              |
| 4:E:275:ARG:NH2    | 4:E:331:ASP:OD2    | 2.39                     | 0.56              |
| 25:AA:919:A:OP1    | 39:AO:92:LYS:NZ    | 2.31                     | 0.56              |
| 25:AA:1398:U:OP1   | 50:AZ:29:LYS:NZ    | 2.29                     | 0.56              |
| 55:A4:302:VAL:HA   | 55:A4:312:LYS:HD2  | 1.88                     | 0.56              |
| 1:A:3175:A:OP2     | 1:A:3187:C:N4      | 2.37                     | 0.56              |
| 48:AX:295:LYS:NZ   | 96:AX:503:GDP:O1A  | 2.38                     | 0.56              |
| 1:A:2194:U:O2'     | 79:I:115:ARG:NH1   | 2.37                     | 0.56              |
| 12:N:123:ARG:O     | 12:N:158:ARG:NH2   | 2.39                     | 0.56              |
| 22:X:118:ILE:O     | 22:X:168:ARG:NH1   | 2.39                     | 0.56              |
| 37:AM:104:ILE:HG23 | 42:AR:147:ILE:HG12 | 1.87                     | 0.56              |
| 44:AT:29:VAL:HB    | 44:AT:79:TYR:HB2   | 1.88                     | 0.56              |
| 73:f:208:LEU:HG    | 73:f:212:LYS:HE3   | 1.88                     | 0.56              |
| 85:s:49:ALA:O      | 85:s:61:ARG:NH1    | 2.39                     | 0.56              |
| 52:A1:235:ASN:ND2  | 52:A1:237:GLU:OE2  | 2.38                     | 0.56              |
| 64:6:139:TRP:O     | 64:6:144:GLY:N     | 2.39                     | 0.56              |
| 69:b:49:ARG:HG3    | 69:b:50:GLU:HG2    | 1.88                     | 0.56              |
| 73:f:122:GLU:N     | 73:f:158:GLN:O     | 2.39                     | 0.56              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:A:2752:C:H2'     | 1:A:2753:A:H8      | 1.71                     | 0.56              |
| 1:A:2804:A:H2'     | 1:A:2805:A:H8      | 1.70                     | 0.56              |
| 14:P:93:LEU:HD21   | 14:P:101:VAL:HG22  | 1.88                     | 0.56              |
| 21:W:148:LEU:HB3   | 82:p:128:ASN:HA    | 1.88                     | 0.56              |
| 25:AA:1235:U:OP1   | 35:AK:36:ARG:NH2   | 2.36                     | 0.56              |
| 26:AB:239:ASN:ND2  | 26:AB:242:SER:OG   | 2.39                     | 0.56              |
| 52:A1:50:ARG:NH1   | 55:A4:94:TYR:O     | 2.39                     | 0.56              |
| 63:5:160:HIS:HA    | 63:5:164:TRP:HB2   | 1.89                     | 0.56              |
| 1:A:2137:C:OP2     | 24:Z:77:ARG:NH1    | 2.39                     | 0.55              |
| 1:A:2175:C:H2'     | 1:A:2176:C:C6      | 2.41                     | 0.55              |
| 17:S:115:LEU:HD11  | 17:S:190:GLN:HB3   | 1.87                     | 0.55              |
| 48:AX:102:ARG:NH1  | 48:AX:132:THR:O    | 2.39                     | 0.55              |
| 49:AY:353:LEU:HD21 | 50:AZ:26:THR:HG21  | 1.87                     | 0.55              |
| 63:5:229:ARG:NH1   | 63:5:231:SER:OG    | 2.39                     | 0.55              |
| 70:c:101:GLU:HG2   | 70:c:117:LEU:HD13  | 1.88                     | 0.55              |
| 78:k:40:GLU:OE1    | 78:k:43:ARG:NH2    | 2.38                     | 0.55              |
| 1:A:2740:A:N3      | 1:A:2921:A:O2'     | 2.34                     | 0.55              |
| 19:U:126:LEU:HD22  | 71:d:76:ILE:HD12   | 1.88                     | 0.55              |
| 25:AA:1003:A:H2'   | 25:AA:1004:G:H8    | 1.71                     | 0.55              |
| 31:AG:70:THR:HG23  | 31:AG:73:PHE:H     | 1.71                     | 0.55              |
| 48:AX:67:HIS:HB3   | 48:AX:98:CYS:HB3   | 1.88                     | 0.55              |
| 1:A:1749:C:O2'     | 11:M:80:LYS:NZ     | 2.32                     | 0.55              |
| 18:T:63:ARG:NH1    | 71:d:228:PHE:O     | 2.39                     | 0.55              |
| 27:AC:84:GLU:OE1   | 27:AC:84:GLU:N     | 2.36                     | 0.55              |
| 42:AR:347:GLN:NE2  | 42:AR:351:GLU:OE2  | 2.39                     | 0.55              |
| 10:L:96:MET:HE1    | 15:Q:121:THR:HG21  | 1.87                     | 0.55              |
| 15:Q:74:ARG:NH2    | 15:Q:287:GLU:OE2   | 2.35                     | 0.55              |
| 25:AA:1528:A:OP1   | 51:A0:101:ARG:NH2  | 2.39                     | 0.55              |
| 51:A0:65:LEU:HD23  | 51:A0:68:LEU:HD12  | 1.89                     | 0.55              |
| 56:Ax:28:C:H42     | 56:Ax:42:G:H1      | 1.54                     | 0.55              |
| 65:7:92:ALA:O      | 65:7:95:LEU:C      | 2.50                     | 0.55              |
| 1:A:2027:A:O2'     | 1:A:2048:U:OP1     | 2.23                     | 0.55              |
| 1:A:2043:C:C2      | 1:A:2044:A:C8      | 2.95                     | 0.55              |
| 4:E:244:ALA:HB1    | 4:E:248:ILE:HD11   | 1.88                     | 0.55              |
| 43:AS:85:PHE:HB2   | 47:AW:100:VAL:HG12 | 1.88                     | 0.55              |
| 48:AX:283:ALA:HB3  | 48:AX:286:GLU:HG3  | 1.89                     | 0.55              |
| 55:A4:611:LEU:HA   | 55:A4:614:LEU:HD12 | 1.89                     | 0.55              |
| 1:A:2353:A:N6      | 1:A:2357:C:OP2     | 2.38                     | 0.55              |
| 1:A:2655:G:N2      | 1:A:2659:C:O2'     | 2.40                     | 0.55              |
| 7:I:188:ARG:HD2    | 78:k:55:VAL:HB     | 1.89                     | 0.55              |
| 35:AK:58:ARG:NE    | 35:AK:72:ASP:OD1   | 2.40                     | 0.55              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 51:A0:68:LEU:HD22  | 51:A0:75:GLY:HA3   | 1.89                     | 0.55              |
| 63:5:105:TYR:CZ    | 63:5:262:ILE:HD12  | 2.41                     | 0.55              |
| 65:7:282:ALA:HB3   | 65:7:298:GLN:HB2   | 1.89                     | 0.55              |
| 80:m:56:LEU:HD23   | 80:m:64:ILE:HD11   | 1.89                     | 0.55              |
| 85:s:316:CYS:HB3   | 85:s:319:GLN:HB2   | 1.88                     | 0.55              |
| 15:Q:233:TRP:HB3   | 15:Q:240:ILE:HD12  | 1.89                     | 0.55              |
| 32:AH:120:LEU:HD21 | 35:AK:101:LYS:HD3  | 1.89                     | 0.55              |
| 47:AW:150:THR:HG22 | 47:AW:161:THR:HB   | 1.89                     | 0.55              |
| 1:A:2740:A:H2'     | 1:A:2741:A:H8      | 1.71                     | 0.55              |
| 1:A:3189:C:O2'     | 84:r:155:ALA:N     | 2.39                     | 0.55              |
| 6:H:94:LEU:HB2     | 6:H:116:LYS:HD3    | 1.89                     | 0.55              |
| 13:O:154:GLN:HG2   | 13:O:157:ARG:HH21  | 1.72                     | 0.55              |
| 63:5:126:THR:HB    | 63:5:372:ASN:HB2   | 1.89                     | 0.55              |
| 64:6:90:ILE:HG13   | 64:6:167:PHE:HB3   | 1.88                     | 0.55              |
| 66:8:99:ARG:HA     | 72:e:84:TYR:HB2    | 1.89                     | 0.55              |
| 1:A:2246:A:H2'     | 1:A:2247:C:H6      | 1.72                     | 0.55              |
| 7:I:75:GLU:O       | 7:I:80:ARG:NH1     | 2.39                     | 0.55              |
| 55:A4:74:LEU:O     | 55:A4:77:THR:OG1   | 2.23                     | 0.55              |
| 69:b:28:ARG:NH1    | 69:b:78:GLU:OE1    | 2.39                     | 0.55              |
| 73:f:101:THR:OG1   | 80:m:67:ARG:NH1    | 2.39                     | 0.55              |
| 4:E:47:THR:HG21    | 65:7:307:ARG:HD2   | 1.89                     | 0.55              |
| 4:E:76:LYS:HG3     | 4:E:170:LEU:HD21   | 1.87                     | 0.55              |
| 13:O:49:VAL:HG11   | 13:O:121:ALA:HB3   | 1.87                     | 0.55              |
| 25:AA:1102:A:OP2   | 25:AA:1104:A:N6    | 2.38                     | 0.55              |
| 32:AH:176:GLN:NE2  | 32:AH:178:GLU:OE2  | 2.38                     | 0.55              |
| 11:M:11:ARG:NH2    | 74:g:142:GLU:OE2   | 2.40                     | 0.54              |
| 17:S:100:HIS:HB2   | 17:S:134:LEU:HD11  | 1.89                     | 0.54              |
| 25:AA:826:A:C6     | 34:AJ:56:PRO:HD2   | 2.41                     | 0.54              |
| 42:AR:219:TYR:O    | 42:AR:256:ARG:NH2  | 2.38                     | 0.54              |
| 55:A4:129:GLN:NE2  | 55:A4:144:TYR:OH   | 2.40                     | 0.54              |
| 10:L:100:PHE:HB3   | 15:Q:158:GLN:HE21  | 1.73                     | 0.54              |
| 25:AA:1162:A:N3    | 25:AA:1497:C:O2'   | 2.39                     | 0.54              |
| 27:AC:86:THR:HG21  | 35:AK:106:LEU:HD11 | 1.88                     | 0.54              |
| 55:A4:156:ALA:HB3  | 55:A4:172:MET:HE1  | 1.89                     | 0.54              |
| 1:A:1749:C:OP2     | 1:A:2899:C:O2'     | 2.22                     | 0.54              |
| 1:A:3046:C:H2'     | 1:A:3047:G:H8      | 1.71                     | 0.54              |
| 28:AD:392:ARG:NH1  | 28:AD:396:GLU:OE2  | 2.40                     | 0.54              |
| 30:AF:74:ILE:HG13  | 31:AG:366:GLN:HA   | 1.90                     | 0.54              |
| 73:f:106:TYR:OH    | 73:f:174:ILE:O     | 2.24                     | 0.54              |
| 1:A:2093:U:O2      | 1:A:2266:U:O2'     | 2.24                     | 0.54              |
| 63:5:119:GLN:NE2   | 63:5:261:PRO:O     | 2.37                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:A:1707:C:N3      | 63:5:80:ARG:NH1    | 2.51                     | 0.54              |
| 1:A:1828:A:H4'     | 1:A:1829:A:C8      | 2.43                     | 0.54              |
| 4:E:210:THR:OG1    | 4:E:262:GLY:O      | 2.22                     | 0.54              |
| 7:I:148:VAL:O      | 78:k:31:ARG:NH2    | 2.40                     | 0.54              |
| 25:AA:1464:G:H21   | 25:AA:1466:C:H41   | 1.55                     | 0.54              |
| 29:AE:37:ARG:NH1   | 29:AE:69:TYR:OH    | 2.41                     | 0.54              |
| 51:A0:163:SER:HB3  | 51:A0:190:MET:HB3  | 1.89                     | 0.54              |
| 63:5:245:ILE:O     | 63:5:248:THR:OG1   | 2.25                     | 0.54              |
| 25:AA:990:U:H3     | 25:AA:997:A:H61    | 1.56                     | 0.54              |
| 46:AV:128:THR:HB   | 46:AV:137:ILE:HG13 | 1.89                     | 0.54              |
| 1:A:1829:A:H2'     | 1:A:1830:G:H8      | 1.72                     | 0.54              |
| 1:A:2795:U:H2'     | 1:A:2796:G:H8      | 1.72                     | 0.54              |
| 25:AA:1239:C:H2'   | 25:AA:1240:A:C8    | 2.42                     | 0.54              |
| 31:AG:196:GLY:O    | 31:AG:248:VAL:N    | 2.41                     | 0.54              |
| 34:AJ:78:ARG:HG3   | 34:AJ:118:LEU:HD21 | 1.90                     | 0.54              |
| 1:A:2694:A:N3      | 1:A:2942:C:O2'     | 2.36                     | 0.54              |
| 14:P:126:GLU:OE1   | 14:P:160:ARG:NH2   | 2.37                     | 0.54              |
| 25:AA:1085:C:OP1   | 33:AI:189:ARG:NH1  | 2.36                     | 0.54              |
| 39:AO:217:ARG:NH1  | 39:AO:227:GLU:OE2  | 2.40                     | 0.54              |
| 44:AT:32:VAL:HG22  | 44:AT:76:LEU:HD22  | 1.88                     | 0.54              |
| 1:A:2454:G:OP1     | 13:O:48:ARG:NH2    | 2.39                     | 0.54              |
| 2:B:74:C:OP1       | 72:e:219:GLN:NE2   | 2.41                     | 0.54              |
| 10:L:93:GLY:O      | 10:L:95:ARG:NH2    | 2.41                     | 0.54              |
| 28:AD:316:CYS:HB3  | 28:AD:334:ALA:HB3  | 1.89                     | 0.54              |
| 48:AX:273:THR:HG23 | 48:AX:316:LEU:HD13 | 1.89                     | 0.54              |
| 72:e:71:ALA:HB2    | 80:m:40:LEU:HD22   | 1.89                     | 0.54              |
| 1:A:2950:U:H2'     | 1:A:2951:A:H8      | 1.73                     | 0.53              |
| 1:A:3200:U:H2'     | 1:A:3201:A:C2      | 2.43                     | 0.53              |
| 1:A:3205:C:OP2     | 4:E:298:LYS:NZ     | 2.35                     | 0.53              |
| 2:B:23:A:H2'       | 2:B:24:G:C8        | 2.44                     | 0.53              |
| 25:AA:701:G:O6     | 51:A0:48:ARG:NH1   | 2.41                     | 0.53              |
| 25:AA:1454:G:OP2   | 31:AG:377:ARG:NH1  | 2.41                     | 0.53              |
| 32:AH:50:LEU:HD22  | 55:A4:80:ARG:HB3   | 1.89                     | 0.53              |
| 42:AR:78:ILE:HG23  | 42:AR:299:ASN:HB3  | 1.90                     | 0.53              |
| 63:5:146:HIS:O     | 63:5:194:LYS:NZ    | 2.41                     | 0.53              |
| 64:6:215:THR:OG1   | 64:6:275:GLN:OE1   | 2.26                     | 0.53              |
| 1:A:2740:A:H2'     | 1:A:2741:A:C8      | 2.42                     | 0.53              |
| 3:D:126:VAL:HA     | 3:D:142:VAL:HG12   | 1.90                     | 0.53              |
| 5:F:94:ASP:OD1     | 81:o:91:GLN:NE2    | 2.42                     | 0.53              |
| 42:AR:70:PHE:O     | 42:AR:76:GLN:NE2   | 2.41                     | 0.53              |
| 55:A4:308:LYS:HE3  | 55:A4:310:GLU:HB3  | 1.90                     | 0.53              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 85:s:89:MET:HE3   | 85:s:275:LYS:HB3   | 1.91                     | 0.53              |
| 1:A:2747:U:H2'    | 1:A:2748:A:H8      | 1.73                     | 0.53              |
| 1:A:3082:G:N2     | 1:A:3085:A:OP2     | 2.27                     | 0.53              |
| 19:U:46:MET:HB3   | 67:9:36:ARG:HB3    | 1.89                     | 0.53              |
| 54:A3:159:GLU:OE2 | 54:A3:163:ARG:NH1  | 2.41                     | 0.53              |
| 10:L:60:VAL:HA    | 10:L:73:ILE:HG22   | 1.91                     | 0.53              |
| 25:AA:1050:C:H2'  | 25:AA:1051:A:C8    | 2.44                     | 0.53              |
| 28:AD:224:GLU:OE2 | 28:AD:226:ARG:NH2  | 2.41                     | 0.53              |
| 29:AE:9:ILE:HD12  | 29:AE:90:ARG:HB2   | 1.89                     | 0.53              |
| 61:3:175:ASP:HB3  | 61:3:178:GLN:HB2   | 1.90                     | 0.53              |
| 73:f:55:GLY:HA3   | 73:f:58:LYS:HE3    | 1.91                     | 0.53              |
| 1:A:2093:U:H4'    | 76:i:126:LYS:HE2   | 1.90                     | 0.53              |
| 1:A:2175:C:H2'    | 1:A:2176:C:H6      | 1.74                     | 0.53              |
| 19:U:74:HIS:HB2   | 67:9:24:LYS:HE3    | 1.91                     | 0.53              |
| 25:AA:889:G:N2    | 25:AA:902:G:OP1    | 2.40                     | 0.53              |
| 25:AA:917:C:O2'   | 25:AA:921:U:OP1    | 2.27                     | 0.53              |
| 25:AA:1046:A:O2'  | 25:AA:1048:C:OP2   | 2.24                     | 0.53              |
| 25:AA:1578:A:H2'  | 25:AA:1579:C:C6    | 2.42                     | 0.53              |
| 32:AH:55:PRO:HA   | 55:A4:440:LYS:HB3  | 1.90                     | 0.53              |
| 42:AR:82:MET:HE3  | 42:AR:288:GLN:HE22 | 1.73                     | 0.53              |
| 1:A:2485:U:H3     | 1:A:2650:C:H42     | 0.72                     | 0.53              |
| 1:A:2491:C:H2'    | 1:A:2492:G:C8      | 2.43                     | 0.53              |
| 8:J:119:GLU:HB3   | 79:l:75:VAL:HG21   | 1.90                     | 0.53              |
| 25:AA:1078:A:OP1  | 56:Ax:38:C:O2'     | 2.24                     | 0.53              |
| 25:AA:1452:U:H2'  | 25:AA:1453:A:H8    | 1.73                     | 0.53              |
| 25:AA:1470:A:H2'  | 25:AA:1471:A:C8    | 2.43                     | 0.53              |
| 26:AB:99:HIS:ND1  | 26:AB:100:ARG:O    | 2.41                     | 0.53              |
| 41:AQ:68:MET:HE2  | 53:A2:29:LEU:HD22  | 1.89                     | 0.53              |
| 48:AX:81:HIS:CD2  | 48:AX:190:ASN:HB3  | 2.44                     | 0.53              |
| 1:A:1780:U:H1'    | 19:U:83:ARG:HH22   | 1.72                     | 0.53              |
| 1:A:1803:A:H4'    | 1:A:1804:A:H3'     | 1.90                     | 0.53              |
| 1:A:2403:G:OP2    | 3:D:105:ARG:NH2    | 2.40                     | 0.53              |
| 1:A:3201:A:H2'    | 1:A:3202:U:O4'     | 2.09                     | 0.53              |
| 25:AA:843:G:N2    | 25:AA:846:A:OP2    | 2.26                     | 0.53              |
| 51:A0:135:MET:N   | 51:A0:135:MET:SD   | 2.81                     | 0.53              |
| 1:A:2586:U:H2'    | 1:A:2587:G:H8      | 1.73                     | 0.53              |
| 6:H:79:VAL:HG22   | 22:X:89:GLN:HB2    | 1.90                     | 0.53              |
| 7:I:119:HIS:CD2   | 7:I:163:GLU:HG2    | 2.44                     | 0.53              |
| 14:P:123:VAL:HG11 | 64:6:128:ALA:HB3   | 1.89                     | 0.53              |
| 25:AA:773:U:H2'   | 25:AA:774:G:C8     | 2.44                     | 0.53              |
| 25:AA:1365:A:H4'  | 25:AA:1389:G:H4'   | 1.90                     | 0.53              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 48:AX:47:ALA:HB1   | 48:AX:50:ARG:HB2  | 1.89                     | 0.53              |
| 56:Ax:4:A:H2'      | 56:Ax:5:A:C8      | 2.43                     | 0.53              |
| 64:6:240:ILE:HG12  | 64:6:248:GLY:HA3  | 1.90                     | 0.53              |
| 1:A:1821:A:OP2     | 58:0:95:ARG:NH1   | 2.41                     | 0.53              |
| 1:A:2086:A:H2'     | 1:A:2087:U:C6     | 2.43                     | 0.53              |
| 1:A:2295:C:OP2     | 16:R:17:ARG:NH2   | 2.40                     | 0.53              |
| 2:B:72:G:C2        | 2:B:73:A:C8       | 2.96                     | 0.53              |
| 46:AV:46:GLU:OE2   | 46:AV:74:ARG:NE   | 2.42                     | 0.53              |
| 51:A0:30:ASP:OD1   | 51:A0:212:ARG:NH2 | 2.35                     | 0.53              |
| 63:5:98:LEU:HD13   | 63:5:272:ASP:HB2  | 1.90                     | 0.53              |
| 1:A:2402:A:H2'     | 3:D:133:PRO:HG3   | 1.90                     | 0.53              |
| 8:J:142:ARG:HH11   | 79:l:99:MET:HE1   | 1.74                     | 0.53              |
| 10:L:94:PRO:O      | 10:L:97:THR:OG1   | 2.22                     | 0.53              |
| 37:AM:21:LEU:HB3   | 37:AM:32:TYR:HB3  | 1.91                     | 0.53              |
| 51:A0:63:ARG:NH2   | 51:A0:110:ASP:OD2 | 2.42                     | 0.53              |
| 64:6:161:LEU:HD13  | 64:6:271:LEU:HD11 | 1.90                     | 0.53              |
| 20:V:36:PRO:HG2    | 20:V:39:ILE:HB    | 1.90                     | 0.52              |
| 25:AA:1347:G:OP1   | 35:AK:36:ARG:NH1  | 2.33                     | 0.52              |
| 25:AA:1396:C:H5''  | 80:m:90:ARG:HE    | 1.73                     | 0.52              |
| 55:A4:525:SER:HA   | 55:A4:528:ARG:HE  | 1.73                     | 0.52              |
| 69:b:26:LEU:HD22   | 69:b:105:ALA:HA   | 1.91                     | 0.52              |
| 1:A:2344:C:H1'     | 1:A:2362:A:H4'    | 1.91                     | 0.52              |
| 7:l:173:PHE:HD1    | 78:k:51:VAL:HB    | 1.73                     | 0.52              |
| 25:AA:663:A:H2'    | 25:AA:664:G:C8    | 2.45                     | 0.52              |
| 25:AA:706:C:OP1    | 51:A0:43:ARG:NE   | 2.42                     | 0.52              |
| 28:AD:294:ILE:HB   | 28:AD:305:MET:HE3 | 1.91                     | 0.52              |
| 39:AO:199:TRP:NE1  | 51:A0:166:TYR:O   | 2.33                     | 0.52              |
| 46:AV:179:GLN:OE1  | 46:AV:215:GLN:NE2 | 2.42                     | 0.52              |
| 46:AV:266:VAL:HG11 | 46:AV:275:LEU:HG  | 1.91                     | 0.52              |
| 65:7:194:PRO:HG3   | 65:7:283:VAL:HB   | 1.90                     | 0.52              |
| 70:c:72:ILE:HD13   | 70:c:178:LEU:HD13 | 1.90                     | 0.52              |
| 81:o:24:PRO:HG2    | 84:r:169:TRP:HB2  | 1.90                     | 0.52              |
| 7:I:102:VAL:HG23   | 7:I:104:LEU:HG    | 1.91                     | 0.52              |
| 13:O:87:PRO:O      | 13:O:91:GLN:HB2   | 2.10                     | 0.52              |
| 26:AB:172:ARG:HB2  | 26:AB:175:MET:HE2 | 1.92                     | 0.52              |
| 46:AV:357:THR:HG22 | 46:AV:361:LYS:HE3 | 1.91                     | 0.52              |
| 1:A:1907:A:OP1     | 5:F:126:LYS:NZ    | 2.33                     | 0.52              |
| 1:A:2347:C:H2'     | 1:A:2348:A:H8     | 1.73                     | 0.52              |
| 11:M:264:GLN:NE2   | 11:M:266:PHE:O    | 2.41                     | 0.52              |
| 25:AA:842:C:N4     | 25:AA:843:G:O6    | 2.42                     | 0.52              |
| 1:A:2407:U:H2'     | 1:A:2408:U:H6     | 1.74                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:A:3152:C:OP1     | 15:Q:141:SER:OG    | 2.24                     | 0.52              |
| 2:B:40:U:H5''      | 14:P:155:SER:HB3   | 1.91                     | 0.52              |
| 19:U:19:VAL:HB     | 67:9:136:LEU:HD23  | 1.90                     | 0.52              |
| 25:AA:1025:A:H2'   | 25:AA:1026:A:C8    | 2.44                     | 0.52              |
| 30:AF:240:ARG:NH1  | 30:AF:242:TRP:OXT  | 2.43                     | 0.52              |
| 32:AH:64:THR:OG1   | 55:A4:64:THR:OG1   | 2.24                     | 0.52              |
| 63:5:162:ARG:NH1   | 63:5:383:TYR:OH    | 2.39                     | 0.52              |
| 72:e:48:LEU:HB2    | 72:e:231:VAL:HG12  | 1.92                     | 0.52              |
| 1:A:2042:U:H2'     | 1:A:2043:C:H6      | 1.75                     | 0.52              |
| 1:A:2192:A:O2'     | 8:J:135:VAL:HG11   | 2.10                     | 0.52              |
| 25:AA:1515:G:H2'   | 25:AA:1516:G:C8    | 2.45                     | 0.52              |
| 29:AE:96:HIS:HB3   | 29:AE:99:THR:HG23  | 1.91                     | 0.52              |
| 59:1:24:ALA:HB2    | 59:1:54:VAL:HG11   | 1.92                     | 0.52              |
| 70:c:245:LEU:HD12  | 70:c:253:PRO:HD3   | 1.92                     | 0.52              |
| 80:m:103:ARG:HB3   | 80:m:108:GLN:HE21  | 1.74                     | 0.52              |
| 1:A:3115:U:H2'     | 1:A:3116:C:H6      | 1.73                     | 0.52              |
| 15:Q:80:PHE:O      | 15:Q:282:ILE:HD13  | 2.09                     | 0.52              |
| 23:Y:171:ASP:OD1   | 23:Y:175:ARG:N     | 2.43                     | 0.52              |
| 25:AA:1415:G:OP2   | 25:AA:1415:G:N2    | 2.20                     | 0.52              |
| 32:AH:79:LEU:HD11  | 32:AH:140:TYR:HB3  | 1.91                     | 0.52              |
| 48:AX:210:TRP:HB2  | 48:AX:214:GLU:HB2  | 1.90                     | 0.52              |
| 72:e:58:VAL:N      | 72:e:153:LEU:O     | 2.41                     | 0.52              |
| 83:q:112:GLN:OE1   | 83:q:115:ARG:NH2   | 2.41                     | 0.52              |
| 1:A:2522:U:H1'     | 63:5:35:VAL:HG12   | 1.90                     | 0.52              |
| 5:F:72:PHE:HA      | 5:F:206:LEU:HD13   | 1.92                     | 0.52              |
| 5:F:211:ARG:HD3    | 75:h:58:ARG:HH21   | 1.75                     | 0.52              |
| 25:AA:740:G:H2'    | 25:AA:741:A:H8     | 1.74                     | 0.52              |
| 25:AA:872:G:H2'    | 25:AA:873:G:H8     | 1.75                     | 0.52              |
| 25:AA:1278:C:H1'   | 26:AB:181:LEU:HD22 | 1.91                     | 0.52              |
| 39:AO:167:ILE:HD12 | 42:AR:230:LEU:HG   | 1.91                     | 0.52              |
| 50:AZ:13:ARG:NH1   | 80:m:109:GLU:O     | 2.43                     | 0.52              |
| 51:A0:167:PRO:HG2  | 51:A0:170:LEU:HB2  | 1.90                     | 0.52              |
| 55:A4:472:ASP:OD1  | 55:A4:505:ARG:NH1  | 2.43                     | 0.52              |
| 1:A:3024:U:H2'     | 1:A:3025:A:H8      | 1.75                     | 0.52              |
| 4:E:148:GLY:HA3    | 4:E:173:LYS:HG3    | 1.92                     | 0.52              |
| 13:O:106:ARG:HE    | 13:O:126:LYS:HE2   | 1.75                     | 0.52              |
| 24:Z:68:ILE:HD11   | 24:Z:122:LEU:HD13  | 1.91                     | 0.52              |
| 25:AA:872:G:H2'    | 25:AA:873:G:C8     | 2.45                     | 0.52              |
| 25:AA:1380:G:N3    | 48:AX:164:ASN:ND2  | 2.55                     | 0.52              |
| 31:AG:263:ASP:OD1  | 31:AG:267:MET:N    | 2.42                     | 0.52              |
| 32:AH:148:LEU:HD13 | 32:AH:153:ALA:HB2  | 1.92                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 42:AR:159:THR:HG23 | 42:AR:172:ILE:HG12 | 1.91                     | 0.52              |
| 52:A1:155:ASP:OD1  | 52:A1:215:ARG:NH1  | 2.31                     | 0.52              |
| 1:A:1750:G:H2'     | 1:A:1751:A:C8      | 2.45                     | 0.52              |
| 1:A:1886:G:N7      | 5:F:170:ARG:NH2    | 2.58                     | 0.52              |
| 1:A:1979:U:H2'     | 1:A:1980:A:C8      | 2.45                     | 0.52              |
| 1:A:2082:G:OP1     | 81:o:66:ARG:NH2    | 2.42                     | 0.52              |
| 1:A:2682:A:H5''    | 16:R:34:ARG:HH21   | 1.74                     | 0.52              |
| 9:K:136:ASP:OD1    | 70:c:264:THR:OG1   | 2.24                     | 0.52              |
| 31:AG:90:ASN:ND2   | 52:A1:62:VAL:O     | 2.43                     | 0.52              |
| 42:AR:157:VAL:HG11 | 42:AR:192:MET:HE3  | 1.91                     | 0.52              |
| 56:Ax:66:C:H2'     | 56:Ax:67:C:H6      | 1.74                     | 0.52              |
| 1:A:3115:U:H2'     | 1:A:3116:C:C6      | 2.45                     | 0.51              |
| 17:S:98:VAL:HB     | 17:S:135:LEU:HB3   | 1.91                     | 0.51              |
| 31:AG:353:CYS:HA   | 31:AG:356:VAL:HG22 | 1.92                     | 0.51              |
| 64:6:216:LEU:HD11  | 64:6:270:PHE:HB3   | 1.93                     | 0.51              |
| 1:A:2160:A:N6      | 62:4:70:THR:O      | 2.40                     | 0.51              |
| 5:F:279:ARG:HH12   | 5:F:282:PRO:HD3    | 1.74                     | 0.51              |
| 33:AI:151:VAL:HG21 | 33:AI:158:ARG:HG3  | 1.93                     | 0.51              |
| 42:AR:281:ILE:HB   | 42:AR:300:LEU:HD21 | 1.90                     | 0.51              |
| 65:7:240:ILE:HG23  | 65:7:252:VAL:HG21  | 1.90                     | 0.51              |
| 1:A:2175:C:H4'     | 8:J:102:ARG:HG2    | 1.90                     | 0.51              |
| 1:A:2187:C:H2'     | 1:A:2188:A:C8      | 2.45                     | 0.51              |
| 1:A:2332:C:H41     | 1:A:2442:U:H3      | 1.58                     | 0.51              |
| 3:D:127:ILE:HD11   | 3:D:143:ALA:HB2    | 1.92                     | 0.51              |
| 22:X:241:GLN:NE2   | 22:X:245:GLU:OE2   | 2.43                     | 0.51              |
| 42:AR:312:GLN:HB2  | 42:AR:335:GLU:HG3  | 1.91                     | 0.51              |
| 55:A4:332:LEU:HD21 | 55:A4:368:SER:HB3  | 1.92                     | 0.51              |
| 72:e:58:VAL:HB     | 72:e:153:LEU:HB3   | 1.91                     | 0.51              |
| 78:k:18:VAL:HG22   | 78:k:64:VAL:HG22   | 1.90                     | 0.51              |
| 1:A:1895:C:H2'     | 1:A:1896:U:H6      | 1.76                     | 0.51              |
| 20:V:54:TRP:NE1    | 20:V:56:LEU:O      | 2.43                     | 0.51              |
| 25:AA:1022:A:OP2   | 53:A2:17:ARG:NE    | 2.42                     | 0.51              |
| 1:A:1829:A:H2'     | 1:A:1830:G:C8      | 2.46                     | 0.51              |
| 1:A:2196:A:O2'     | 1:A:2213:A:N1      | 2.42                     | 0.51              |
| 1:A:2530:A:H5''    | 3:D:212:THR:HG21   | 1.92                     | 0.51              |
| 5:F:195:LEU:HD22   | 5:F:202:TYR:HE2    | 1.75                     | 0.51              |
| 47:AW:126:ARG:NH1  | 47:AW:131:GLY:O    | 2.34                     | 0.51              |
| 48:AX:369:GLU:HG3  | 48:AX:370:LYS:HG2  | 1.93                     | 0.51              |
| 73:f:48:TYR:HB3    | 73:f:51:LYS:HG2    | 1.93                     | 0.51              |
| 25:AA:1211:G:H2'   | 25:AA:1212:U:C6    | 2.46                     | 0.51              |
| 25:AA:1272:A:N1    | 25:AA:1303:G:O2'   | 2.43                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 40:AP:124:TYR:HE2  | 41:AQ:4:HIS:HB3    | 1.75                     | 0.51              |
| 50:AZ:18:LEU:HD21  | 80:m:114:LEU:HD11  | 1.92                     | 0.51              |
| 56:Ax:27:U:H2'     | 56:Ax:28:C:C6      | 2.45                     | 0.51              |
| 1:A:1911:C:H2'     | 1:A:1912:A:H8      | 1.75                     | 0.51              |
| 1:A:2017:U:OP2     | 11:M:59:ARG:NH2    | 2.41                     | 0.51              |
| 46:AV:250:ILE:HB   | 51:A0:146:GLU:HG3  | 1.91                     | 0.51              |
| 19:U:48:MET:HE2    | 19:U:53:LEU:HA     | 1.93                     | 0.51              |
| 23:Y:187:PRO:HD2   | 23:Y:190:LEU:HD12  | 1.91                     | 0.51              |
| 25:AA:1456:U:OP1   | 31:AG:338:SER:OG   | 2.25                     | 0.51              |
| 31:AG:165:VAL:HG11 | 31:AG:224:LEU:HB3  | 1.93                     | 0.51              |
| 46:AV:236:LEU:HD12 | 46:AV:290:LEU:HD13 | 1.92                     | 0.51              |
| 55:A4:345:PHE:HB3  | 55:A4:348:PHE:HD2  | 1.76                     | 0.51              |
| 65:7:247:ASN:ND2   | 65:7:251:ILE:HG12  | 2.26                     | 0.51              |
| 67:9:16:ASP:N      | 67:9:16:ASP:OD1    | 2.44                     | 0.51              |
| 1:A:1789:A:N3      | 1:A:1915:C:O2'     | 2.40                     | 0.51              |
| 8:J:25:ARG:NH1     | 79:l:58:ASP:OD1    | 2.31                     | 0.51              |
| 8:J:101:ALA:HB1    | 8:J:107:GLU:HG3    | 1.92                     | 0.51              |
| 13:O:33:LEU:HD21   | 13:O:59:LEU:HD22   | 1.93                     | 0.51              |
| 13:O:64:LYS:NZ     | 13:O:100:GLN:O     | 2.43                     | 0.51              |
| 24:Z:120:LYS:NZ    | 81:o:44:GLU:OE2    | 2.38                     | 0.51              |
| 35:AK:34:MET:HE3   | 35:AK:95:SER:HB2   | 1.92                     | 0.51              |
| 45:AU:168:ILE:HG12 | 45:AU:176:ARG:HG3  | 1.93                     | 0.51              |
| 52:A1:56:ARG:HG3   | 52:A1:60:MET:HE3   | 1.93                     | 0.51              |
| 72:e:54:GLN:HG2    | 72:e:158:VAL:HG22  | 1.92                     | 0.51              |
| 2:B:21:A:OP2       | 64:6:106:ARG:NH1   | 2.41                     | 0.51              |
| 5:F:212:TRP:O      | 5:F:258:THR:OG1    | 2.25                     | 0.51              |
| 27:AC:126:GLN:O    | 52:A1:49:ARG:NH2   | 2.44                     | 0.51              |
| 48:AX:163:LYS:HB3  | 48:AX:316:LEU:HD11 | 1.92                     | 0.51              |
| 63:5:354:PHE:HB3   | 63:5:417:LEU:HD11  | 1.93                     | 0.51              |
| 73:f:127:MET:HB2   | 73:f:154:GLU:HB3   | 1.93                     | 0.51              |
| 1:A:2310:G:N2      | 1:A:2676:A:OP2     | 2.35                     | 0.50              |
| 1:A:2803:A:H2'     | 1:A:2804:A:O4'     | 2.11                     | 0.50              |
| 5:F:94:ASP:OD1     | 5:F:94:ASP:N       | 2.34                     | 0.50              |
| 7:I:76:ILE:HG22    | 7:I:78:LEU:H       | 1.76                     | 0.50              |
| 7:I:140:TYR:HB3    | 7:I:143:LEU:HD12   | 1.91                     | 0.50              |
| 35:AK:52:LEU:HD11  | 50:AZ:36:LEU:HB3   | 1.92                     | 0.50              |
| 77:j:53:ASP:OD2    | 77:j:55:ARG:NH2    | 2.43                     | 0.50              |
| 1:A:2442:U:OP1     | 85:s:81:ARG:NH2    | 2.30                     | 0.50              |
| 5:F:62:VAL:HG23    | 5:F:82:LEU:HB2     | 1.93                     | 0.50              |
| 10:L:98:PRO:HA     | 15:Q:162:ILE:HG12  | 1.91                     | 0.50              |
| 16:R:16:ASP:OD1    | 16:R:16:ASP:N      | 2.40                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 21:W:102:GLU:OE2   | 64:6:74:TYR:N      | 2.44                     | 0.50              |
| 55:A4:516:SER:HB3  | 55:A4:521:HIS:HB2  | 1.92                     | 0.50              |
| 74:g:150:LYS:NZ    | 81:o:79:THR:O      | 2.43                     | 0.50              |
| 1:A:1897:A:H2'     | 1:A:1898:A:C8      | 2.46                     | 0.50              |
| 25:AA:1042:U:H2'   | 25:AA:1043:C:H6    | 1.76                     | 0.50              |
| 25:AA:1471:A:H2'   | 25:AA:1472:G:H8    | 1.75                     | 0.50              |
| 32:AH:65:ILE:HG12  | 55:A4:63:LYS:HG2   | 1.93                     | 0.50              |
| 38:AN:29:ARG:HD3   | 38:AN:46:ARG:HD2   | 1.94                     | 0.50              |
| 55:A4:526:ASP:OD1  | 55:A4:527:LEU:N    | 2.44                     | 0.50              |
| 64:6:236:LEU:HB3   | 64:6:252:CYS:HB3   | 1.94                     | 0.50              |
| 69:b:48:GLU:OE2    | 81:o:101:TRP:NE1   | 2.39                     | 0.50              |
| 1:A:1742:G:O2'     | 1:A:1754:G:O6      | 2.28                     | 0.50              |
| 1:A:2457:A:O2'     | 13:O:17:ARG:NH1    | 2.43                     | 0.50              |
| 1:A:2673:G:H5''    | 18:T:106:LYS:HB2   | 1.93                     | 0.50              |
| 1:A:3019:G:O2'     | 1:A:3125:A:N1      | 2.43                     | 0.50              |
| 63:5:177:CYS:HB3   | 63:5:178:PRO:HD3   | 1.92                     | 0.50              |
| 64:6:311:MET:O     | 77:j:112:LYS:NZ    | 2.44                     | 0.50              |
| 1:A:2051:A:H2'     | 1:A:2052:A:C8      | 2.47                     | 0.50              |
| 2:B:29:C:H2'       | 2:B:30:A:H8        | 1.76                     | 0.50              |
| 25:AA:889:G:N1     | 25:AA:905:A:OP2    | 2.35                     | 0.50              |
| 32:AH:164:LEU:HD12 | 32:AH:165:PRO:HD2  | 1.92                     | 0.50              |
| 54:A3:174:ARG:HA   | 54:A3:177:TRP:CE2  | 2.46                     | 0.50              |
| 56:Ax:22:A:H2'     | 56:Ax:23:G:H8      | 1.76                     | 0.50              |
| 73:f:172:GLU:OE1   | 73:f:175:GLN:NE2   | 2.44                     | 0.50              |
| 1:A:2215:C:OP2     | 12:N:31:LYS:NZ     | 2.44                     | 0.50              |
| 1:A:2335:A:H2'     | 1:A:2336:U:H6      | 1.76                     | 0.50              |
| 1:A:2416:U:H3      | 85:s:166:TYR:HD1   | 1.59                     | 0.50              |
| 18:T:150:ILE:HB    | 71:d:52:THR:HG21   | 1.92                     | 0.50              |
| 32:AH:64:THR:HG1   | 55:A4:64:THR:HG1   | 1.50                     | 0.50              |
| 54:A3:170:GLU:OE2  | 54:A3:193:LYS:NZ   | 2.45                     | 0.50              |
| 64:6:198:ALA:O     | 64:6:254:TYR:OH    | 2.28                     | 0.50              |
| 71:d:200:SER:HB2   | 71:d:204:ASN:HD21  | 1.77                     | 0.50              |
| 76:i:57:TYR:OH     | 83:q:28:ARG:O      | 2.23                     | 0.50              |
| 1:A:1787:G:N2      | 1:A:1790:A:OP2     | 2.28                     | 0.50              |
| 1:A:3231:U:H3      | 13:O:106:ARG:HG2   | 1.76                     | 0.50              |
| 18:T:185:THR:HG23  | 18:T:188:ALA:H     | 1.77                     | 0.50              |
| 23:Y:85:TRP:HH2    | 67:9:70:LEU:HD22   | 1.76                     | 0.50              |
| 25:AA:798:C:H2'    | 25:AA:799:A:C8     | 2.47                     | 0.50              |
| 28:AD:380:LEU:HD12 | 28:AD:381:PRO:HD2  | 1.94                     | 0.50              |
| 37:AM:67:ALA:HB1   | 42:AR:161:ILE:HD13 | 1.93                     | 0.50              |
| 53:A2:49:MET:HG2   | 53:A2:53:MET:HE2   | 1.93                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 73:f:90:VAL:HG11   | 73:f:158:GLN:HE21  | 1.77                     | 0.50              |
| 1:A:2246:A:H2'     | 1:A:2247:C:C6      | 2.47                     | 0.50              |
| 1:A:2727:C:H2'     | 1:A:2728:C:C6      | 2.47                     | 0.50              |
| 25:AA:916:C:H2'    | 25:AA:917:C:C6     | 2.46                     | 0.50              |
| 25:AA:1411:G:H2'   | 25:AA:1412:G:H8    | 1.77                     | 0.50              |
| 55:A4:531:ILE:HG22 | 55:A4:535:MET:HE2  | 1.94                     | 0.50              |
| 64:6:188:TYR:OH    | 82:p:190:GLN:NE2   | 2.45                     | 0.50              |
| 6:H:62:VAL:HG22    | 6:H:77:HIS:HD2     | 1.77                     | 0.50              |
| 17:S:131:GLU:HB3   | 17:S:151:LYS:HE2   | 1.93                     | 0.50              |
| 21:W:100:THR:OG1   | 21:W:132:HIS:NE2   | 2.36                     | 0.50              |
| 25:AA:1595:G:H2'   | 25:AA:1596:A:C8    | 2.47                     | 0.50              |
| 29:AE:15:ARG:NH2   | 45:AU:182:ASP:OD1  | 2.45                     | 0.50              |
| 46:AV:270:PRO:O    | 46:AV:346:LYS:NZ   | 2.45                     | 0.50              |
| 1:A:2321:A:OP1     | 58:0:138:ARG:NH1   | 2.45                     | 0.49              |
| 1:A:2321:A:N1      | 58:0:142:GLY:HA3   | 2.27                     | 0.49              |
| 12:N:218:ILE:HG23  | 12:N:223:MET:HB2   | 1.93                     | 0.49              |
| 25:AA:684:U:H2'    | 25:AA:685:A:H8     | 1.76                     | 0.49              |
| 46:AV:139:PRO:HB2  | 46:AV:143:THR:HB   | 1.94                     | 0.49              |
| 46:AV:240:LEU:HD22 | 46:AV:253:PRO:HB3  | 1.93                     | 0.49              |
| 55:A4:596:LEU:HD11 | 55:A4:614:LEU:HD11 | 1.94                     | 0.49              |
| 84:r:37:GLU:OE1    | 84:r:52:ARG:NH2    | 2.44                     | 0.49              |
| 1:A:2816:G:O6      | 21:W:33:LYS:NZ     | 2.44                     | 0.49              |
| 3:D:204:ALA:O      | 3:D:208:ARG:NH2    | 2.37                     | 0.49              |
| 14:P:51:ARG:NH2    | 64:6:221:LEU:O     | 2.44                     | 0.49              |
| 31:AG:209:LEU:O    | 31:AG:211:GLU:N    | 2.39                     | 0.49              |
| 46:AV:331:LEU:HG   | 46:AV:335:LYS:HE3  | 1.94                     | 0.49              |
| 80:m:79:ILE:HD11   | 80:m:84:LEU:HD21   | 1.94                     | 0.49              |
| 1:A:1789:A:H2'     | 1:A:1790:A:C8      | 2.46                     | 0.49              |
| 1:A:1792:G:OP2     | 60:2:85:LYS:NZ     | 2.45                     | 0.49              |
| 1:A:1907:A:N3      | 1:A:2930:U:O2'     | 2.43                     | 0.49              |
| 1:A:2236:C:N4      | 1:A:2688:C:O2      | 2.45                     | 0.49              |
| 29:AE:40:GLU:HB2   | 29:AE:65:LEU:HB2   | 1.94                     | 0.49              |
| 46:AV:29:LEU:N     | 46:AV:149:ASP:OD1  | 2.44                     | 0.49              |
| 48:AX:79:PHE:HZ    | 48:AX:143:HIS:HB2  | 1.76                     | 0.49              |
| 48:AX:126:LEU:HD23 | 48:AX:343:ILE:HB   | 1.93                     | 0.49              |
| 72:e:45:TRP:CD2    | 72:e:230:LYS:HE3   | 2.47                     | 0.49              |
| 1:A:1822:U:O2      | 1:A:2707:A:O2'     | 2.30                     | 0.49              |
| 1:A:1939:G:O2'     | 1:A:1973:G:H4'     | 2.12                     | 0.49              |
| 1:A:2380:C:H5''    | 1:A:2381:A:OP2     | 2.12                     | 0.49              |
| 1:A:3051:A:H2'     | 1:A:3052:A:C8      | 2.47                     | 0.49              |
| 2:B:44:A:OP1       | 64:6:114:ARG:NH2   | 2.45                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:J:25:ARG:HD2     | 79:l:56:LEU:HB3    | 1.94                     | 0.49              |
| 16:R:108:TYR:HD1   | 69:b:125:SER:HB2   | 1.77                     | 0.49              |
| 25:AA:1056:A:H4'   | 25:AA:1588:G:N2    | 2.26                     | 0.49              |
| 25:AA:1201:A:H2'   | 25:AA:1202:G:C8    | 2.47                     | 0.49              |
| 28:AD:203:LEU:HD21 | 28:AD:222:ILE:HD11 | 1.94                     | 0.49              |
| 37:AM:74:ARG:NH2   | 45:AU:77:GLU:OE1   | 2.45                     | 0.49              |
| 48:AX:207:LYS:HB2  | 48:AX:218:LYS:HB2  | 1.93                     | 0.49              |
| 73:f:137:LEU:HA    | 73:f:144:MET:HA    | 1.94                     | 0.49              |
| 25:AA:769:G:OP2    | 38:AN:73:ARG:NH2   | 2.45                     | 0.49              |
| 25:AA:1007:G:H2'   | 25:AA:1008:A:C8    | 2.48                     | 0.49              |
| 25:AA:1527:A:H2'   | 25:AA:1528:A:O4'   | 2.13                     | 0.49              |
| 55:A4:513:TRP:HB2  | 55:A4:531:ILE:HD13 | 1.94                     | 0.49              |
| 61:3:168:ARG:NH1   | 61:3:170:ASN:OD1   | 2.45                     | 0.49              |
| 64:6:155:TYR:O     | 64:6:267:ARG:NH1   | 2.45                     | 0.49              |
| 1:A:1812:C:OP1     | 18:T:44:LYS:NZ     | 2.40                     | 0.49              |
| 1:A:2734:A:H2'     | 1:A:2735:G:H8      | 1.77                     | 0.49              |
| 10:L:35:MET:O      | 10:L:56:ARG:NH1    | 2.46                     | 0.49              |
| 25:AA:1129:U:H2'   | 25:AA:1130:G:H8    | 1.76                     | 0.49              |
| 1:A:2727:C:H2'     | 1:A:2728:C:H6      | 1.78                     | 0.49              |
| 1:A:2751:G:H2'     | 1:A:2752:C:C6      | 2.48                     | 0.49              |
| 4:E:221:ARG:NH1    | 4:E:257:MET:O      | 2.43                     | 0.49              |
| 25:AA:1308:U:H2'   | 25:AA:1309:A:H8    | 1.78                     | 0.49              |
| 25:AA:1462:G:H2'   | 25:AA:1463:G:H8    | 1.77                     | 0.49              |
| 42:AR:209:ILE:HA   | 42:AR:214:ASN:HD22 | 1.77                     | 0.49              |
| 47:AW:103:ARG:HG2  | 47:AW:139:ARG:HG2  | 1.94                     | 0.49              |
| 63:5:165:GLN:HG2   | 63:5:166:THR:HG23  | 1.95                     | 0.49              |
| 63:5:242:ARG:NH2   | 63:5:337:GLU:O     | 2.45                     | 0.49              |
| 1:A:1980:A:OP1     | 60:2:56:SER:OG     | 2.31                     | 0.49              |
| 1:A:2612:C:O2'     | 25:AA:1503:G:O2'   | 2.30                     | 0.49              |
| 10:L:43:ASN:OD1    | 10:L:118:ARG:N     | 2.45                     | 0.49              |
| 25:AA:1302:C:OP1   | 27:AC:165:LYS:NZ   | 2.39                     | 0.49              |
| 36:AL:128:ARG:HH21 | 36:AL:166:MET:HE2  | 1.76                     | 0.49              |
| 55:A4:598:LEU:O    | 55:A4:602:HIS:ND1  | 2.39                     | 0.49              |
| 71:d:203:MET:H     | 71:d:208:VAL:HG22  | 1.78                     | 0.49              |
| 1:A:2746:U:H2'     | 1:A:2747:U:C6      | 2.48                     | 0.49              |
| 31:AG:202:LYS:O    | 31:AG:206:GLU:HG2  | 2.13                     | 0.49              |
| 42:AR:262:LEU:O    | 42:AR:265:THR:OG1  | 2.25                     | 0.49              |
| 43:AS:104:THR:HG22 | 43:AS:108:LYS:HE2  | 1.95                     | 0.49              |
| 56:Ax:69:U:H2'     | 56:Ax:70:A:C8      | 2.48                     | 0.49              |
| 85:s:152:GLN:NE2   | 85:s:179:GLN:OE1   | 2.46                     | 0.49              |
| 1:A:1834:U:C4      | 18:T:200:ARG:HA    | 2.48                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:Y:154:ARG:HA    | 67:9:130:LEU:HD13  | 1.95                     | 0.49              |
| 25:AA:769:G:N2     | 25:AA:772:A:OP2    | 2.44                     | 0.49              |
| 25:AA:1439:A:H2'   | 25:AA:1440:G:H8    | 1.78                     | 0.49              |
| 25:AA:1471:A:H2'   | 25:AA:1472:G:C8    | 2.47                     | 0.49              |
| 48:AX:365:TRP:NE1  | 48:AX:395:CYS:O    | 2.46                     | 0.49              |
| 70:c:140:PHE:HB3   | 70:c:314:TRP:HH2   | 1.77                     | 0.49              |
| 74:g:154:ASP:N     | 74:g:154:ASP:OD1   | 2.46                     | 0.49              |
| 1:A:2443:C:O2      | 1:A:2444:A:N6      | 2.46                     | 0.48              |
| 1:A:2616:A:O2'     | 1:A:3046:C:O2      | 2.30                     | 0.48              |
| 1:A:3089:A:H5'     | 56:Ax:74:C:H5''    | 1.95                     | 0.48              |
| 18:T:138:GLU:HB2   | 18:T:171:LYS:HB3   | 1.95                     | 0.48              |
| 25:AA:1118:A:H4'   | 28:AD:355:ARG:HH12 | 1.76                     | 0.48              |
| 26:AB:222:ILE:HD13 | 26:AB:236:VAL:HB   | 1.94                     | 0.48              |
| 53:A2:100:LEU:HB3  | 53:A2:103:LYS:HG2  | 1.95                     | 0.48              |
| 70:c:72:ILE:HG23   | 70:c:88:LEU:HD23   | 1.95                     | 0.48              |
| 85:s:204:CYS:SG    | 85:s:240:GLN:NE2   | 2.86                     | 0.48              |
| 1:A:2099:U:H2'     | 1:A:2100:C:C6      | 2.47                     | 0.48              |
| 1:A:2392:U:H2'     | 1:A:2394:A:H62     | 1.78                     | 0.48              |
| 1:A:3230:G:N7      | 4:E:156:ARG:NH2    | 2.60                     | 0.48              |
| 6:H:141:GLU:HA     | 6:H:144:LYS:HE2    | 1.94                     | 0.48              |
| 25:AA:798:C:H2'    | 25:AA:799:A:H8     | 1.79                     | 0.48              |
| 32:AH:121:LEU:HD21 | 32:AH:128:LYS:HD2  | 1.95                     | 0.48              |
| 55:A4:308:LYS:HG3  | 55:A4:311:GLU:H    | 1.78                     | 0.48              |
| 56:Ax:66:C:H2'     | 56:Ax:67:C:C6      | 2.47                     | 0.48              |
| 63:5:276:ASP:OD2   | 85:s:160:ARG:NH2   | 2.46                     | 0.48              |
| 64:6:162:PHE:HB3   | 64:6:165:ALA:HB3   | 1.95                     | 0.48              |
| 64:6:244:ARG:NH1   | 64:6:247:GLU:OE1   | 2.46                     | 0.48              |
| 65:7:176:SER:O     | 65:7:319:ARG:NH2   | 2.46                     | 0.48              |
| 81:o:71:PHE:CE2    | 81:o:75:LYS:HD2    | 2.47                     | 0.48              |
| 1:A:1860:A:H5''    | 1:A:2681:G:H5''    | 1.94                     | 0.48              |
| 15:Q:177:VAL:HG11  | 15:Q:204:MET:HG3   | 1.94                     | 0.48              |
| 23:Y:202:LEU:HB2   | 23:Y:204:TYR:CE2   | 2.47                     | 0.48              |
| 25:AA:1144:U:H2'   | 25:AA:1145:A:H8    | 1.78                     | 0.48              |
| 33:AI:121:LYS:H    | 33:AI:121:LYS:HD2  | 1.78                     | 0.48              |
| 67:9:68:PHE:CE2    | 67:9:70:LEU:HB2    | 2.48                     | 0.48              |
| 85:s:248:ALA:HB2   | 85:s:430:LYS:HG3   | 1.96                     | 0.48              |
| 1:A:1979:U:H2'     | 1:A:1980:A:H8      | 1.78                     | 0.48              |
| 1:A:2468:A:H61     | 1:A:2659:C:H42     | 1.60                     | 0.48              |
| 11:M:73:PRO:HG2    | 11:M:76:ILE:HB     | 1.96                     | 0.48              |
| 13:O:29:LEU:HD22   | 13:O:52:MET:HB3    | 1.94                     | 0.48              |
| 18:T:42:SER:O      | 18:T:43:ARG:NH1    | 2.41                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:AA:844:A:H4'    | 45:AU:64:ARG:HH12  | 1.79                     | 0.48              |
| 25:AA:1003:A:H2'   | 25:AA:1004:G:C8    | 2.48                     | 0.48              |
| 31:AG:255:GLN:HG2  | 31:AG:370:LEU:HD13 | 1.96                     | 0.48              |
| 32:AH:53:ASP:OD2   | 55:A4:80:ARG:NH1   | 2.46                     | 0.48              |
| 36:AL:175:TYR:HB2  | 38:AN:89:GLY:HA3   | 1.96                     | 0.48              |
| 48:AX:162:VAL:HB   | 48:AX:272:THR:HB   | 1.96                     | 0.48              |
| 49:AY:349:HIS:CD2  | 50:AZ:24:ARG:HD2   | 2.48                     | 0.48              |
| 51:A0:41:LEU:HD13  | 51:A0:55:TRP:CG    | 2.49                     | 0.48              |
| 63:5:229:ARG:NH2   | 63:5:286:PRO:O     | 2.45                     | 0.48              |
| 73:f:136:GLN:HG2   | 80:m:78:PRO:HG3    | 1.94                     | 0.48              |
| 1:A:2485:U:O2      | 1:A:2650:C:N3      | 2.46                     | 0.48              |
| 1:A:3202:U:OP2     | 4:E:141:LYS:NZ     | 2.43                     | 0.48              |
| 3:D:113:ARG:O      | 3:D:147:ARG:NH1    | 2.37                     | 0.48              |
| 5:F:114:THR:O      | 5:F:156:ARG:NH1    | 2.46                     | 0.48              |
| 12:N:33:LEU:HD22   | 79:l:125:ASN:HD22  | 1.78                     | 0.48              |
| 19:U:44:ILE:HG13   | 19:U:93:LYS:HB3    | 1.95                     | 0.48              |
| 25:AA:1050:C:H2'   | 25:AA:1051:A:H8    | 1.78                     | 0.48              |
| 25:AA:1134:G:OP2   | 34:AJ:38:ARG:NH2   | 2.46                     | 0.48              |
| 28:AD:296:LEU:HD11 | 28:AD:303:ILE:HD12 | 1.95                     | 0.48              |
| 31:AG:197:SER:O    | 31:AG:245:ARG:NH2  | 2.45                     | 0.48              |
| 42:AR:195:VAL:HG22 | 42:AR:204:ILE:HD13 | 1.96                     | 0.48              |
| 83:q:40:PRO:HG2    | 83:q:51:GLN:HB3    | 1.95                     | 0.48              |
| 1:A:2081:U:O2      | 24:Z:109:LYS:NZ    | 2.45                     | 0.48              |
| 1:A:2431:C:OP2     | 1:A:2433:C:N4      | 2.38                     | 0.48              |
| 1:A:2900:C:H2'     | 1:A:2901:A:H8      | 1.79                     | 0.48              |
| 1:A:3110:C:O2'     | 4:E:266:ARG:NH1    | 2.46                     | 0.48              |
| 1:A:3144:A:H2'     | 1:A:3145:A:H8      | 1.78                     | 0.48              |
| 3:D:111:ARG:NH2    | 3:D:165:ASN:OD1    | 2.35                     | 0.48              |
| 8:J:159:LEU:HD21   | 8:J:164:LEU:HD13   | 1.94                     | 0.48              |
| 25:AA:1149:G:OP2   | 54:A3:165:LYS:NZ   | 2.39                     | 0.48              |
| 25:AA:1408:A:H2'   | 25:AA:1409:A:H8    | 1.79                     | 0.48              |
| 44:AT:132:ARG:NH1  | 44:AT:136:LEU:O    | 2.45                     | 0.48              |
| 56:Ax:8:U:H5'      | 56:Ax:49:G:H5'     | 1.95                     | 0.48              |
| 63:5:283:TYR:HE1   | 85:s:152:GLN:HB2   | 1.78                     | 0.48              |
| 1:A:2668:A:H2'     | 1:A:2669:A:C8      | 2.48                     | 0.48              |
| 2:B:55:U:C4        | 2:B:56:U:H1'       | 2.49                     | 0.48              |
| 7:I:168:LEU:HD13   | 7:I:176:LEU:HB2    | 1.96                     | 0.48              |
| 19:U:20:PHE:O      | 23:Y:99:HIS:NE2    | 2.34                     | 0.48              |
| 20:V:63:GLU:HB2    | 20:V:73:GLN:HG2    | 1.96                     | 0.48              |
| 20:V:122:LEU:HD21  | 20:V:154:ILE:HG21  | 1.95                     | 0.48              |
| 25:AA:705:C:H5'    | 51:A0:51:PRO:HG3   | 1.96                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:AG:276:ARG:HG3  | 31:AG:277:LYS:H    | 1.78                     | 0.48              |
| 76:i:83:TRP:HZ3    | 76:i:90:ARG:HG2    | 1.79                     | 0.48              |
| 1:A:2016:C:OP2     | 11:M:59:ARG:NH1    | 2.47                     | 0.48              |
| 1:A:2039:A:N6      | 1:A:2729:U:O2      | 2.47                     | 0.48              |
| 1:A:2795:U:H2'     | 1:A:2796:G:C8      | 2.48                     | 0.48              |
| 3:D:289:LEU:HD12   | 3:D:290:PRO:HD2    | 1.95                     | 0.48              |
| 25:AA:715:G:H2'    | 25:AA:716:U:C6     | 2.49                     | 0.48              |
| 25:AA:799:A:H2'    | 25:AA:800:C:C6     | 2.48                     | 0.48              |
| 25:AA:1174:U:H2'   | 25:AA:1175:G:H8    | 1.79                     | 0.48              |
| 26:AB:138:ARG:HB3  | 43:AS:30:LEU:HD11  | 1.95                     | 0.48              |
| 47:AW:114:ILE:HD13 | 47:AW:140:VAL:HG21 | 1.96                     | 0.48              |
| 52:A1:86:ARG:HB3   | 52:A1:96:PRO:HB2   | 1.95                     | 0.48              |
| 1:A:1673:U:O2'     | 18:T:143:ARG:NH1   | 2.46                     | 0.48              |
| 1:A:2051:A:H2'     | 1:A:2052:A:H8      | 1.78                     | 0.48              |
| 1:A:2176:C:H5'     | 8:J:102:ARG:HH22   | 1.77                     | 0.48              |
| 1:A:3165:C:H2'     | 1:A:3166:U:C6      | 2.49                     | 0.48              |
| 12:N:103:GLU:OE1   | 12:N:106:ARG:NH2   | 2.37                     | 0.48              |
| 25:AA:1118:A:H4'   | 28:AD:351:ARG:HH21 | 1.77                     | 0.48              |
| 37:AM:63:GLU:HG2   | 42:AR:155:LYS:HE2  | 1.96                     | 0.48              |
| 39:AO:105:CYS:HB2  | 39:AO:142:VAL:HA   | 1.96                     | 0.48              |
| 46:AV:116:CYS:HA   | 46:AV:121:ALA:HB3  | 1.95                     | 0.48              |
| 49:AY:315:ILE:HD12 | 52:A1:157:VAL:HG13 | 1.96                     | 0.48              |
| 1:A:2167:A:N6      | 1:A:2212:C:OP2     | 2.47                     | 0.48              |
| 20:V:19:TYR:OH     | 20:V:31:ASP:OD2    | 2.29                     | 0.48              |
| 25:AA:686:A:H2'    | 25:AA:687:G:H8     | 1.79                     | 0.48              |
| 44:AT:47:PHE:HD1   | 44:AT:51:ASN:HD22  | 1.62                     | 0.48              |
| 46:AV:187:PHE:HD1  | 46:AV:190:LEU:HD12 | 1.78                     | 0.48              |
| 56:Ax:27:U:H2'     | 56:Ax:28:C:H6      | 1.79                     | 0.48              |
| 65:7:155:GLU:HA    | 65:7:164:VAL:HG11  | 1.95                     | 0.48              |
| 84:r:124:ARG:NH1   | 84:r:153:ARG:O     | 2.45                     | 0.48              |
| 1:A:1760:G:OP2     | 83:q:55:ARG:NH2    | 2.47                     | 0.47              |
| 4:E:345:ILE:O      | 15:Q:172:GLN:NE2   | 2.47                     | 0.47              |
| 25:AA:1456:U:H2'   | 25:AA:1457:G:O4'   | 2.15                     | 0.47              |
| 25:AA:1462:G:H2'   | 25:AA:1463:G:C8    | 2.48                     | 0.47              |
| 37:AM:54:TYR:HD1   | 37:AM:66:VAL:HG22  | 1.77                     | 0.47              |
| 1:A:2075:U:O2'     | 1:A:2833:A:N7      | 2.41                     | 0.47              |
| 22:X:226:LEU:HD12  | 23:Y:155:LEU:HB3   | 1.94                     | 0.47              |
| 25:AA:686:A:H2'    | 25:AA:687:G:C8     | 2.48                     | 0.47              |
| 25:AA:1529:A:O2'   | 46:AV:64:LYS:O     | 2.30                     | 0.47              |
| 28:AD:148:LEU:HD21 | 55:A4:108:LEU:HB2  | 1.96                     | 0.47              |
| 65:7:247:ASN:HD21  | 65:7:249:GLU:HB2   | 1.78                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:A:2318:A:H2'     | 1:A:2319:A:C8      | 2.50                     | 0.47              |
| 1:A:2804:A:H2'     | 1:A:2805:A:C8      | 2.48                     | 0.47              |
| 11:M:146:ASP:HA    | 82:p:144:PHE:HE1   | 1.78                     | 0.47              |
| 25:AA:700:A:N1     | 25:AA:709:G:O2'    | 2.41                     | 0.47              |
| 25:AA:1006:U:H2'   | 25:AA:1007:G:H8    | 1.78                     | 0.47              |
| 25:AA:1298:U:H4'   | 26:AB:172:ARG:HH21 | 1.78                     | 0.47              |
| 25:AA:1504:U:H2'   | 25:AA:1505:A:C8    | 2.50                     | 0.47              |
| 35:AK:53:ARG:O     | 35:AK:56:SER:OG    | 2.29                     | 0.47              |
| 46:AV:95:PHE:O     | 46:AV:98:SER:OG    | 2.26                     | 0.47              |
| 48:AX:138:LEU:HD11 | 48:AX:261:ALA:HB1  | 1.96                     | 0.47              |
| 48:AX:153:LEU:HD21 | 48:AX:244:LEU:HD22 | 1.96                     | 0.47              |
| 55:A4:331:ASN:HD21 | 55:A4:333:GLN:HB2  | 1.79                     | 0.47              |
| 1:A:2598:A:H3'     | 1:A:2625:C:H42     | 1.79                     | 0.47              |
| 1:A:3144:A:H2'     | 1:A:3145:A:C8      | 2.49                     | 0.47              |
| 4:E:210:THR:HG22   | 4:E:290:PRO:HB3    | 1.95                     | 0.47              |
| 8:J:114:LEU:HD13   | 79:l:97:PHE:HA     | 1.97                     | 0.47              |
| 9:K:22:ASP:HB3     | 9:K:147:GLN:HE21   | 1.78                     | 0.47              |
| 19:U:29:VAL:HG12   | 23:Y:117:GLN:HG2   | 1.96                     | 0.47              |
| 25:AA:806:C:OP2    | 25:AA:807:A:N6     | 2.30                     | 0.47              |
| 30:AF:161:ILE:HD12 | 30:AF:170:VAL:HG21 | 1.96                     | 0.47              |
| 33:AI:163:HIS:NE2  | 41:AQ:20:GLU:OE2   | 2.47                     | 0.47              |
| 73:f:93:ILE:HG12   | 73:f:186:VAL:HG22  | 1.96                     | 0.47              |
| 1:A:2481:A:H2'     | 1:A:2482:A:C8      | 2.50                     | 0.47              |
| 2:B:74:C:H2'       | 2:B:75:C:O4'       | 2.14                     | 0.47              |
| 10:L:52:HIS:HD2    | 10:L:53:ARG:HG3    | 1.80                     | 0.47              |
| 13:O:133:LEU:HD23  | 58:0:130:VAL:HG11  | 1.95                     | 0.47              |
| 20:V:34:LYS:HG2    | 20:V:35:ASN:H      | 1.79                     | 0.47              |
| 22:X:6:TYR:CG      | 22:X:14:LEU:HD11   | 2.49                     | 0.47              |
| 24:Z:75:THR:HB     | 24:Z:83:LYS:HG2    | 1.96                     | 0.47              |
| 25:AA:1572:A:H2'   | 25:AA:1573:A:C8    | 2.49                     | 0.47              |
| 28:AD:425:LEU:HB3  | 39:AO:88:GLN:HE22  | 1.79                     | 0.47              |
| 42:AR:254:ASP:OD1  | 42:AR:259:TYR:OH   | 2.32                     | 0.47              |
| 47:AW:104:ILE:HG12 | 47:AW:114:ILE:HG12 | 1.96                     | 0.47              |
| 55:A4:152:ILE:HA   | 55:A4:172:MET:HE3  | 1.96                     | 0.47              |
| 76:i:79:TRP:CD1    | 76:i:80:LEU:HG     | 2.50                     | 0.47              |
| 85:s:211:VAL:HG22  | 85:s:230:ARG:HG2   | 1.96                     | 0.47              |
| 1:A:2071:U:O2'     | 64:6:28:ARG:NH2    | 2.47                     | 0.47              |
| 2:B:8:U:O2         | 2:B:15:A:N6        | 2.47                     | 0.47              |
| 3:D:124:GLU:HG2    | 3:D:144:GLY:HA3    | 1.97                     | 0.47              |
| 20:V:48:PRO:HG3    | 23:Y:234:LEU:HD21  | 1.97                     | 0.47              |
| 25:AA:829:C:H1'    | 25:AA:857:G:H22    | 1.79                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:AA:1337:U:H2'   | 25:AA:1338:A:H8    | 1.79                     | 0.47              |
| 42:AR:167:HIS:HB3  | 42:AR:193:ILE:HD13 | 1.96                     | 0.47              |
| 46:AV:251:TRP:HH2  | 51:A0:142:VAL:HG22 | 1.80                     | 0.47              |
| 52:A1:264:GLU:HG2  | 52:A1:268:GLN:HE21 | 1.80                     | 0.47              |
| 64:6:173:LEU:HD13  | 64:6:272:LEU:HD22  | 1.96                     | 0.47              |
| 85:s:332:LEU:HD13  | 85:s:372:TYR:HB2   | 1.96                     | 0.47              |
| 1:A:1977:U:H2'     | 1:A:1978:A:H8      | 1.79                     | 0.47              |
| 1:A:2151:A:O3'     | 81:o:38:ARG:NH2    | 2.47                     | 0.47              |
| 1:A:2245:A:H4'     | 1:A:2246:A:OP1     | 2.13                     | 0.47              |
| 1:A:2336:U:C2      | 1:A:2337:A:C8      | 3.03                     | 0.47              |
| 2:B:12:U:O2'       | 2:B:14:A:OP1       | 2.31                     | 0.47              |
| 18:T:134:LEU:HD23  | 18:T:174:GLU:HA    | 1.95                     | 0.47              |
| 25:AA:661:C:H2'    | 25:AA:662:U:C6     | 2.50                     | 0.47              |
| 25:AA:982:A:H2'    | 25:AA:983:C:H6     | 1.80                     | 0.47              |
| 28:AD:147:PRO:O    | 28:AD:155:GLN:NE2  | 2.48                     | 0.47              |
| 33:AI:100:VAL:HG12 | 33:AI:106:PRO:HA   | 1.95                     | 0.47              |
| 39:AO:96:ARG:HG3   | 39:AO:97:ARG:HG3   | 1.97                     | 0.47              |
| 41:AQ:72:ILE:HD13  | 53:A2:104:LEU:HD21 | 1.96                     | 0.47              |
| 64:6:204:VAL:HG11  | 64:6:216:LEU:HD22  | 1.97                     | 0.47              |
| 74:g:85:PHE:N      | 74:g:114:GLU:O     | 2.47                     | 0.47              |
| 31:AG:161:LEU:HD22 | 31:AG:209:LEU:HD21 | 1.96                     | 0.47              |
| 1:A:1755:A:O2'     | 6:H:64:LEU:O       | 2.29                     | 0.47              |
| 1:A:2491:C:H2'     | 1:A:2492:G:H8      | 1.80                     | 0.47              |
| 1:A:2933:G:N2      | 1:A:2936:U:O2      | 2.43                     | 0.47              |
| 22:X:42:HIS:CG     | 22:X:86:ILE:HD11   | 2.50                     | 0.47              |
| 25:AA:1049:A:H5''  | 36:AL:198:ARG:HB2  | 1.97                     | 0.47              |
| 25:AA:1217:G:H21   | 32:AH:126:ILE:HG22 | 1.79                     | 0.47              |
| 31:AG:285:VAL:HG22 | 31:AG:328:VAL:HG22 | 1.97                     | 0.47              |
| 32:AH:106:ILE:HD11 | 32:AH:143:LEU:HD23 | 1.97                     | 0.47              |
| 38:AN:57:GLN:O     | 38:AN:87:LYS:NZ    | 2.48                     | 0.47              |
| 64:6:303:PHE:HA    | 64:6:306:LYS:HE2   | 1.97                     | 0.47              |
| 82:p:110:TRP:H     | 82:p:110:TRP:CD1   | 2.33                     | 0.47              |
| 1:A:1718:A:N3      | 1:A:1911:C:O2'     | 2.41                     | 0.47              |
| 7:I:100:GLN:HB2    | 7:I:177:LEU:HD11   | 1.96                     | 0.47              |
| 19:U:71:ARG:NH1    | 19:U:73:GLN:OE1    | 2.44                     | 0.47              |
| 55:A4:318:GLU:OE2  | 55:A4:322:HIS:NE2  | 2.48                     | 0.47              |
| 56:Ax:4:A:H2'      | 56:Ax:5:A:H8       | 1.80                     | 0.47              |
| 70:c:93:VAL:HG11   | 70:c:119:LEU:HG    | 1.97                     | 0.47              |
| 73:f:84:THR:H      | 73:f:87:GLU:HB2    | 1.80                     | 0.47              |
| 1:A:1889:C:OP1     | 11:M:133:LYS:NZ    | 2.48                     | 0.46              |
| 1:A:1911:C:H2'     | 1:A:1912:A:C8      | 2.49                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:A:3078:C:N4      | 1:A:3079:G:O6      | 2.48                     | 0.46              |
| 17:S:164:THR:HG22  | 17:S:165:GLU:H     | 1.80                     | 0.46              |
| 19:U:69:ARG:HH22   | 19:U:98:GLN:HE21   | 1.63                     | 0.46              |
| 23:Y:98:LEU:HB3    | 23:Y:142:LEU:HD21  | 1.97                     | 0.46              |
| 25:AA:1106:C:O2'   | 25:AA:1108:C:OP2   | 2.23                     | 0.46              |
| 25:AA:1523:A:H5''  | 46:AV:68:SER:N     | 2.30                     | 0.46              |
| 32:AH:76:LEU:HD22  | 32:AH:174:LYS:HD3  | 1.95                     | 0.46              |
| 52:A1:177:LEU:HB2  | 52:A1:187:LYS:HZ2  | 1.80                     | 0.46              |
| 72:e:160:LEU:HD11  | 72:e:260:LEU:HD12  | 1.97                     | 0.46              |
| 1:A:2115:U:H2'     | 1:A:2116:C:H6      | 1.80                     | 0.46              |
| 1:A:2389:C:P       | 63:5:301:PRO:HB3   | 2.55                     | 0.46              |
| 23:Y:191:ASN:HB3   | 23:Y:194:TYR:HB3   | 1.97                     | 0.46              |
| 25:AA:1201:A:O2'   | 25:AA:1417:A:N3    | 2.38                     | 0.46              |
| 25:AA:1237:A:O2'   | 25:AA:1254:C:O2'   | 2.23                     | 0.46              |
| 25:AA:1578:A:H2'   | 25:AA:1579:C:H6    | 1.80                     | 0.46              |
| 71:d:197:VAL:HG22  | 71:d:212:ILE:HG23  | 1.97                     | 0.46              |
| 72:e:55:ARG:NH1    | 72:e:149:LEU:O     | 2.48                     | 0.46              |
| 80:m:58:LYS:HA     | 80:m:77:MET:HE2    | 1.96                     | 0.46              |
| 85:s:298:GLN:HG3   | 85:s:335:TRP:CZ3   | 2.51                     | 0.46              |
| 1:A:2708:C:O2'     | 58:0:96:ASN:OD1    | 2.23                     | 0.46              |
| 8:J:104:THR:OG1    | 8:J:149:ARG:O      | 2.33                     | 0.46              |
| 13:O:131:PRO:HD3   | 58:0:137:ILE:HD12  | 1.98                     | 0.46              |
| 25:AA:974:U:O2'    | 25:AA:975:A:N7     | 2.47                     | 0.46              |
| 25:AA:1525:C:H5    | 46:AV:103:TYR:HA   | 1.79                     | 0.46              |
| 52:A1:136:ALA:HB3  | 55:A4:57:VAL:HG12  | 1.97                     | 0.46              |
| 55:A4:438:LEU:O    | 55:A4:441:THR:OG1  | 2.33                     | 0.46              |
| 64:6:187:VAL:HG13  | 64:6:319:PHE:HB3   | 1.97                     | 0.46              |
| 80:m:69:ARG:HG3    | 80:m:70:GLU:HG3    | 1.97                     | 0.46              |
| 1:A:3213:A:H2'     | 1:A:3214:C:C6      | 2.49                     | 0.46              |
| 25:AA:1422:G:H2'   | 25:AA:1423:A:C8    | 2.51                     | 0.46              |
| 39:AO:105:CYS:SG   | 39:AO:108:CYS:CB   | 2.92                     | 0.46              |
| 66:8:167:ASN:O     | 72:e:203:LYS:NZ    | 2.48                     | 0.46              |
| 82:p:104:HIS:HA    | 82:p:132:GLU:HA    | 1.96                     | 0.46              |
| 83:q:89:GLU:HA     | 83:q:93:TYR:HD2    | 1.80                     | 0.46              |
| 7:I:146:LEU:HD22   | 78:k:22:PRO:HB2    | 1.97                     | 0.46              |
| 13:O:52:MET:HA     | 13:O:55:TYR:HD2    | 1.79                     | 0.46              |
| 15:Q:62:ILE:HD13   | 46:AV:87:HIS:CD2   | 2.50                     | 0.46              |
| 20:V:122:LEU:HD22  | 20:V:133:ILE:HD11  | 1.98                     | 0.46              |
| 25:AA:649:A:H3'    | 28:AD:335:LYS:HE2  | 1.97                     | 0.46              |
| 30:AF:85:VAL:HB    | 48:AX:370:LYS:HG3  | 1.97                     | 0.46              |
| 55:A4:170:VAL:HG23 | 55:A4:247:ILE:HD11 | 1.98                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 55:A4:452:GLN:HG2  | 55:A4:453:HIS:HD2  | 1.81                     | 0.46              |
| 63:5:99:TYR:HD1    | 63:5:270:ILE:HG12  | 1.81                     | 0.46              |
| 82:p:56:ASP:O      | 82:p:60:ARG:HG3    | 2.15                     | 0.46              |
| 10:L:108:ILE:HA    | 10:L:114:PRO:HA    | 1.98                     | 0.46              |
| 25:AA:1035:U:H2'   | 25:AA:1036:A:C8    | 2.50                     | 0.46              |
| 25:AA:1341:C:OP1   | 50:AZ:100:LYS:N    | 2.49                     | 0.46              |
| 55:A4:598:LEU:HD22 | 55:A4:602:HIS:HE1  | 1.80                     | 0.46              |
| 70:c:42:GLN:HG3    | 76:i:38:LEU:HG     | 1.98                     | 0.46              |
| 1:A:1747:G:OP2     | 1:A:1749:C:N4      | 2.47                     | 0.46              |
| 1:A:1839:C:H2'     | 1:A:1840:C:C6      | 2.50                     | 0.46              |
| 1:A:2065:A:C4      | 1:A:2066:C:C5      | 3.04                     | 0.46              |
| 1:A:2170:G:H2'     | 1:A:2171:U:C5      | 2.51                     | 0.46              |
| 1:A:2950:U:H2'     | 1:A:2951:A:C8      | 2.50                     | 0.46              |
| 4:E:80:LEU:HD12    | 4:E:323:GLY:HA3    | 1.97                     | 0.46              |
| 10:L:126:SER:O     | 10:L:129:LYS:HG2   | 2.16                     | 0.46              |
| 25:AA:1488:5MC:O2  | 25:AA:1584:MA6:O2' | 2.27                     | 0.46              |
| 28:AD:317:HIS:HD2  | 28:AD:318:ARG:H    | 1.63                     | 0.46              |
| 40:AP:115:GLN:HB3  | 40:AP:122:VAL:HG22 | 1.97                     | 0.46              |
| 46:AV:40:TRP:HE1   | 46:AV:111:THR:HG23 | 1.81                     | 0.46              |
| 46:AV:263:MET:HB2  | 46:AV:337:LEU:HD13 | 1.97                     | 0.46              |
| 64:6:120:GLU:OE2   | 66:8:119:LYS:NZ    | 2.48                     | 0.46              |
| 71:d:153:ASN:ND2   | 71:d:183:TRP:H     | 2.14                     | 0.46              |
| 7:I:96:ILE:HA      | 7:I:155:VAL:HG12   | 1.96                     | 0.46              |
| 13:O:130:LEU:HD22  | 58:O:134:THR:HG23  | 1.97                     | 0.46              |
| 15:Q:152:ARG:NH1   | 15:Q:161:GLU:OE2   | 2.48                     | 0.46              |
| 22:X:166:LEU:HD13  | 22:X:196:ILE:HD11  | 1.98                     | 0.46              |
| 25:AA:867:C:H2'    | 25:AA:870:C:H42    | 1.80                     | 0.46              |
| 25:AA:982:A:H2'    | 25:AA:983:C:C6     | 2.51                     | 0.46              |
| 25:AA:1483:C:O2    | 25:AA:1567:A:N6    | 2.49                     | 0.46              |
| 42:AR:281:ILE:HD12 | 42:AR:300:LEU:HG   | 1.98                     | 0.46              |
| 46:AV:276:CYS:HA   | 46:AV:348:GLU:HB3  | 1.98                     | 0.46              |
| 51:A0:129:ARG:NH1  | 51:A0:205:ALA:O    | 2.42                     | 0.46              |
| 55:A4:336:ASN:OD1  | 55:A4:371:THR:OG1  | 2.32                     | 0.46              |
| 62:4:90:VAL:O      | 62:4:99:LYS:HA     | 2.16                     | 0.46              |
| 71:d:153:ASN:ND2   | 71:d:183:TRP:O     | 2.46                     | 0.46              |
| 81:o:15:ARG:HB3    | 81:o:18:ILE:HG12   | 1.98                     | 0.46              |
| 85:s:66:TRP:O      | 85:s:69:THR:OG1    | 2.27                     | 0.46              |
| 16:R:85:ALA:O      | 16:R:89:ASN:ND2    | 2.31                     | 0.46              |
| 19:U:136:GLN:HE22  | 71:d:83:GLY:HA3    | 1.80                     | 0.46              |
| 25:AA:1407:U:H2'   | 25:AA:1408:A:H8    | 1.81                     | 0.46              |
| 46:AV:364:LEU:HG   | 46:AV:368:GLU:HG3  | 1.98                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 51:A0:91:GLU:HB2   | 51:A0:121:LYS:HA   | 1.98                     | 0.46              |
| 56:Ax:41:C:H2'     | 56:Ax:42:G:C8      | 2.51                     | 0.46              |
| 63:5:108:HIS:CE1   | 63:5:110:ARG:HB3   | 2.51                     | 0.46              |
| 65:7:298:GLN:HE22  | 65:7:323:MET:HA    | 1.80                     | 0.46              |
| 66:8:67:ARG:HG2    | 66:8:71:LYS:HE3    | 1.98                     | 0.46              |
| 73:f:104:GLU:HG2   | 73:f:155:ARG:HE    | 1.80                     | 0.46              |
| 1:A:1917:A:N1      | 1:A:1997:C:H1'     | 2.30                     | 0.46              |
| 1:A:2586:U:H2'     | 1:A:2587:G:C8      | 2.50                     | 0.46              |
| 25:AA:1188:A:H4'   | 25:AA:1189:U:H5'   | 1.98                     | 0.46              |
| 39:AO:95:ILE:HG12  | 39:AO:100:VAL:HG12 | 1.98                     | 0.46              |
| 42:AR:231:CYS:SG   | 42:AR:242:TYR:HA   | 2.56                     | 0.46              |
| 48:AX:266:ASN:HB3  | 48:AX:310:LEU:HD22 | 1.98                     | 0.46              |
| 50:AZ:46:LYS:HA    | 50:AZ:49:TYR:CE2   | 2.51                     | 0.46              |
| 65:7:262:ASP:OD1   | 65:7:263:VAL:N     | 2.49                     | 0.46              |
| 85:s:307:ARG:HG3   | 85:s:310:ARG:H     | 1.81                     | 0.46              |
| 1:A:1912:A:H2'     | 1:A:1913:G:C8      | 2.51                     | 0.45              |
| 1:A:2845:A:H2'     | 1:A:2846:G:C8      | 2.52                     | 0.45              |
| 7:I:93:ASN:HA      | 7:I:157:GLU:HA     | 1.97                     | 0.45              |
| 25:AA:649:A:O2'    | 25:AA:651:A:OP2    | 2.32                     | 0.45              |
| 25:AA:702:C:H2'    | 25:AA:703:A:O4'    | 2.16                     | 0.45              |
| 25:AA:1353:A:H5'   | 25:AA:1354:A:C8    | 2.50                     | 0.45              |
| 31:AG:172:LEU:HD11 | 31:AG:237:GLU:HG2  | 1.98                     | 0.45              |
| 42:AR:144:GLU:HG2  | 42:AR:180:THR:HG23 | 1.98                     | 0.45              |
| 48:AX:116:SER:HB3  | 48:AX:119:TYR:HD2  | 1.81                     | 0.45              |
| 66:8:171:PHE:HB3   | 73:f:186:VAL:HB    | 1.98                     | 0.45              |
| 72:e:248:ASN:HA    | 72:e:252:HIS:HE1   | 1.81                     | 0.45              |
| 1:A:1953:A:O2'     | 1:A:2463:A:OP1     | 2.33                     | 0.45              |
| 6:H:65:ALA:HB2     | 6:H:71:PRO:HA      | 1.98                     | 0.45              |
| 9:K:140:ASN:HB2    | 70:c:262:GLY:HA2   | 1.97                     | 0.45              |
| 9:K:169:LEU:HD22   | 84:r:75:TRP:CD1    | 2.51                     | 0.45              |
| 17:S:79:VAL:HA     | 17:S:82:LYS:HE2    | 1.98                     | 0.45              |
| 20:V:105:ARG:NH2   | 71:d:171:ASP:OD1   | 2.49                     | 0.45              |
| 25:AA:818:C:C2     | 25:AA:819:A:C8     | 3.04                     | 0.45              |
| 25:AA:1174:U:H2'   | 25:AA:1175:G:C8    | 2.50                     | 0.45              |
| 25:AA:1561:C:H2'   | 25:AA:1562:G:C8    | 2.51                     | 0.45              |
| 27:AC:104:LEU:HD23 | 27:AC:123:VAL:HG12 | 1.98                     | 0.45              |
| 34:AJ:102:LEU:HD21 | 34:AJ:132:CYS:HA   | 1.98                     | 0.45              |
| 46:AV:225:LEU:HD11 | 46:AV:283:LEU:HD22 | 1.98                     | 0.45              |
| 67:9:115:GLU:HG2   | 67:9:121:PRO:HD3   | 1.98                     | 0.45              |
| 83:q:37:PRO:HG2    | 83:q:68:SER:HA     | 1.96                     | 0.45              |
| 1:A:2192:A:H4'     | 8:J:139:SER:HB3    | 1.97                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 14:P:142:ASN:OD1   | 82:p:184:ASN:ND2   | 2.42                     | 0.45              |
| 25:AA:1512:A:N6    | 25:AA:1536:A:O4'   | 2.49                     | 0.45              |
| 28:AD:282:ILE:HG13 | 28:AD:327:ILE:HD13 | 1.98                     | 0.45              |
| 31:AG:240:PHE:HA   | 31:AG:243:ARG:HD3  | 1.98                     | 0.45              |
| 53:A2:94:GLY:C     | 53:A2:95:GLU:HG3   | 2.41                     | 0.45              |
| 65:7:193:MET:HE3   | 65:7:194:PRO:HD2   | 1.98                     | 0.45              |
| 1:A:1928:A:H2'     | 1:A:1929:A:H8      | 1.80                     | 0.45              |
| 1:A:2187:C:H2'     | 1:A:2188:A:H8      | 1.80                     | 0.45              |
| 1:A:2869:A:OP1     | 61:3:127:ALA:N     | 2.43                     | 0.45              |
| 7:I:100:GLN:HA     | 7:I:151:ASN:HD22   | 1.81                     | 0.45              |
| 25:AA:1007:G:H2'   | 25:AA:1008:A:H8    | 1.81                     | 0.45              |
| 25:AA:1047:A:H2'   | 25:AA:1047:A:N3    | 2.32                     | 0.45              |
| 25:AA:1376:C:H4'   | 25:AA:1377:C:H5'   | 1.98                     | 0.45              |
| 25:AA:1485:G:H2'   | 25:AA:1486:B8T:O4' | 2.17                     | 0.45              |
| 39:AO:94:CYS:HB2   | 39:AO:108:CYS:SG   | 2.56                     | 0.45              |
| 64:6:199:ALA:HA    | 64:6:256:PRO:HB3   | 1.99                     | 0.45              |
| 83:q:55:ARG:HE     | 83:q:59:LYS:HE3    | 1.81                     | 0.45              |
| 85:s:90:LYS:HD2    | 85:s:232:GLN:HB2   | 1.98                     | 0.45              |
| 1:A:1862:U:H2'     | 1:A:1863:A:H8      | 1.81                     | 0.45              |
| 1:A:2016:C:H2'     | 1:A:2017:U:C6      | 2.51                     | 0.45              |
| 1:A:2930:U:H2'     | 1:A:2931:A:H8      | 1.82                     | 0.45              |
| 65:7:78:VAL:HB     | 71:d:282:ILE:HB    | 1.99                     | 0.45              |
| 70:c:93:VAL:HG22   | 70:c:180:LEU:HD12  | 1.99                     | 0.45              |
| 82:p:78:THR:HB     | 82:p:102:ARG:HG3   | 1.99                     | 0.45              |
| 1:A:2081:U:H2'     | 1:A:2082:G:C8      | 2.52                     | 0.45              |
| 7:I:185:ILE:HG22   | 86:t:51:ALA:HB2    | 1.98                     | 0.45              |
| 10:L:86:ILE:HA     | 10:L:105:VAL:HG12  | 1.98                     | 0.45              |
| 12:N:64:ARG:NH1    | 12:N:144:LYS:O     | 2.49                     | 0.45              |
| 25:AA:1399:A:H2'   | 25:AA:1400:U:H6    | 1.81                     | 0.45              |
| 25:AA:1457:G:H5''  | 30:AF:104:LYS:HD2  | 1.98                     | 0.45              |
| 27:AC:100:PHE:HB3  | 27:AC:103:CYS:HB2  | 1.98                     | 0.45              |
| 43:AS:113:ASP:HB2  | 43:AS:116:LYS:HB3  | 1.99                     | 0.45              |
| 48:AX:203:LYS:HA   | 48:AX:221:PRO:HA   | 1.98                     | 0.45              |
| 48:AX:245:LYS:HE2  | 48:AX:249:ARG:HH21 | 1.82                     | 0.45              |
| 56:Ax:65:C:H2'     | 56:Ax:66:C:C6      | 2.51                     | 0.45              |
| 80:m:82:ASP:O      | 80:m:89:ARG:NH2    | 2.49                     | 0.45              |
| 1:A:1698:C:O2'     | 1:A:1702:A:N3      | 2.40                     | 0.45              |
| 1:A:1790:A:OP1     | 60:2:82:ARG:NH1    | 2.49                     | 0.45              |
| 1:A:1831:G:O6      | 69:b:4:ARG:NH2     | 2.48                     | 0.45              |
| 1:A:2060:A:C8      | 1:A:2079:C:C4      | 3.05                     | 0.45              |
| 1:A:2898:U:O2'     | 61:3:113:ARG:NH2   | 2.38                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:A:3139:G:H2'     | 1:A:3140:A:C8      | 2.52                     | 0.45              |
| 3:D:110:LEU:HD22   | 63:5:30:ALA:HB2    | 1.99                     | 0.45              |
| 3:D:184:LEU:HD13   | 3:D:226:ILE:HD11   | 1.99                     | 0.45              |
| 3:D:246:ARG:HH21   | 3:D:250:VAL:HG13   | 1.82                     | 0.45              |
| 4:E:155:PHE:HA     | 65:7:309:HIS:CE1   | 2.52                     | 0.45              |
| 7:I:176:LEU:HD23   | 7:I:188:ARG:HG3    | 1.98                     | 0.45              |
| 23:Y:95:ASN:OD1    | 23:Y:149:ARG:NH1   | 2.50                     | 0.45              |
| 25:AA:1317:A:H3'   | 25:AA:1318:A:H8    | 1.80                     | 0.45              |
| 25:AA:1577:U:H2'   | 25:AA:1578:A:C8    | 2.52                     | 0.45              |
| 30:AF:151:ASN:O    | 30:AF:223:LYS:NZ   | 2.40                     | 0.45              |
| 32:AH:123:SER:OG   | 32:AH:124:VAL:N    | 2.49                     | 0.45              |
| 39:AO:136:TYR:HD2  | 39:AO:138:PRO:HD2  | 1.82                     | 0.45              |
| 66:8:145:GLU:HG2   | 72:e:212:HIS:HE1   | 1.81                     | 0.45              |
| 77:j:91:TRP:CD2    | 81:o:58:GLN:HG2    | 2.51                     | 0.45              |
| 1:A:2725:A:H5'     | 71:d:40:ARG:HH22   | 1.81                     | 0.45              |
| 1:A:2794:C:H2'     | 1:A:2795:U:H6      | 1.81                     | 0.45              |
| 1:A:3181:U:OP1     | 84:r:94:ARG:NH2    | 2.48                     | 0.45              |
| 13:O:80:LEU:HD12   | 13:O:86:ILE:HG12   | 1.98                     | 0.45              |
| 37:AM:55:ASP:OD2   | 44:AT:146:GLN:NE2  | 2.50                     | 0.45              |
| 38:AN:67:ARG:NH1   | 38:AN:80:GLU:OE2   | 2.50                     | 0.45              |
| 66:8:188:PRO:HG2   | 80:m:78:PRO:HB3    | 1.99                     | 0.45              |
| 1:A:1856:A:OP2     | 1:A:2986:C:O2'     | 2.35                     | 0.45              |
| 1:A:2118:U:C2      | 1:A:2119:U:C5      | 3.05                     | 0.45              |
| 1:A:3155:C:H2'     | 1:A:3156:A:C8      | 2.52                     | 0.45              |
| 1:A:3172:C:H1'     | 1:A:3173:G:N2      | 2.32                     | 0.45              |
| 25:AA:748:G:H2'    | 25:AA:749:G:H8     | 1.82                     | 0.45              |
| 25:AA:1399:A:H2'   | 25:AA:1400:U:C6    | 2.52                     | 0.45              |
| 29:AE:31:ASP:OD1   | 45:AU:170:ARG:NH2  | 2.50                     | 0.45              |
| 47:AW:140:VAL:HG12 | 47:AW:172:ILE:HG12 | 1.99                     | 0.45              |
| 85:s:153:GLU:HG3   | 85:s:176:PHE:HB2   | 1.99                     | 0.45              |
| 1:A:2380:C:O2'     | 67:9:46:SER:HB3    | 2.17                     | 0.45              |
| 1:A:2894:U:H5''    | 1:A:2895:U:O4'     | 2.16                     | 0.45              |
| 8:J:101:ALA:HB2    | 8:J:109:ALA:HB2    | 1.99                     | 0.45              |
| 10:L:52:HIS:CD2    | 10:L:53:ARG:HG3    | 2.51                     | 0.45              |
| 25:AA:1194:C:H2'   | 25:AA:1195:U:C6    | 2.51                     | 0.45              |
| 25:AA:1265:C:O2'   | 32:AH:123:SER:HB2  | 2.17                     | 0.45              |
| 28:AD:380:LEU:HB2  | 42:AR:91:PHE:CD2   | 2.52                     | 0.45              |
| 35:AK:56:SER:O     | 35:AK:60:ASN:ND2   | 2.50                     | 0.45              |
| 51:A0:73:LEU:O     | 51:A0:76:LEU:HG    | 2.17                     | 0.45              |
| 64:6:234:HIS:CE1   | 64:6:257:PRO:HA    | 2.52                     | 0.45              |
| 65:7:192:TRP:O     | 65:7:295:ARG:NH2   | 2.50                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 66:8:147:LEU:HB3   | 66:8:158:HIS:HE1   | 1.82                     | 0.45              |
| 66:8:182:ILE:H     | 80:m:61:GLY:HA3    | 1.81                     | 0.45              |
| 1:A:1737:A:O2'     | 76:i:93:ARG:NH2    | 2.44                     | 0.44              |
| 1:A:2230:A:H62     | 1:A:2975:G:H1'     | 1.81                     | 0.44              |
| 1:A:2746:U:H2'     | 1:A:2747:U:H6      | 1.82                     | 0.44              |
| 22:X:40:PRO:HB3    | 22:X:43:TYR:CZ     | 2.52                     | 0.44              |
| 25:AA:1006:U:H2'   | 25:AA:1007:G:C8    | 2.52                     | 0.44              |
| 25:AA:1541:U:H2'   | 25:AA:1542:U:C6    | 2.52                     | 0.44              |
| 33:AI:147:ILE:HG21 | 33:AI:170:LEU:HD13 | 1.99                     | 0.44              |
| 48:AX:189:LYS:HE2  | 48:AX:230:ILE:HG23 | 1.99                     | 0.44              |
| 55:A4:414:LYS:HG2  | 55:A4:453:HIS:CE1  | 2.52                     | 0.44              |
| 64:6:51:TYR:OH     | 64:6:60:ARG:HG2    | 2.17                     | 0.44              |
| 70:c:57:PRO:HB2    | 70:c:184:PHE:HE2   | 1.82                     | 0.44              |
| 72:e:146:ARG:HH11  | 72:e:263:TYR:HE2   | 1.64                     | 0.44              |
| 72:e:159:LEU:HD11  | 72:e:252:HIS:HB2   | 1.99                     | 0.44              |
| 1:A:3009:C:O2'     | 1:A:3115:U:OP1     | 2.31                     | 0.44              |
| 6:H:78:ARG:NH1     | 22:X:87:LEU:O      | 2.50                     | 0.44              |
| 25:AA:740:G:H2'    | 25:AA:741:A:C8     | 2.50                     | 0.44              |
| 46:AV:50:LEU:HD13  | 46:AV:84:GLU:HB3   | 1.97                     | 0.44              |
| 46:AV:117:LEU:HD23 | 46:AV:122:GLN:HG2  | 2.00                     | 0.44              |
| 49:AY:329:HIS:CE1  | 49:AY:330:GLU:HG3  | 2.52                     | 0.44              |
| 59:1:19:ARG:HB2    | 59:1:62:ILE:HD11   | 1.98                     | 0.44              |
| 65:7:51:GLU:HG2    | 65:7:221:VAL:HG12  | 1.98                     | 0.44              |
| 1:A:1863:A:H2'     | 1:A:1864:A:H8      | 1.83                     | 0.44              |
| 2:B:75:C:C4        | 72:e:216:LYS:HB2   | 2.52                     | 0.44              |
| 15:Q:96:ARG:NH2    | 15:Q:285:GLU:HB3   | 2.30                     | 0.44              |
| 20:V:56:LEU:HD13   | 20:V:86:VAL:HG21   | 1.99                     | 0.44              |
| 25:AA:1227:G:H1'   | 32:AH:125:HIS:CD2  | 2.53                     | 0.44              |
| 25:AA:1416:A:H2'   | 25:AA:1417:A:C8    | 2.53                     | 0.44              |
| 30:AF:170:VAL:HG13 | 30:AF:237:ALA:HA   | 1.99                     | 0.44              |
| 32:AH:61:PRO:HG3   | 55:A4:73:ALA:HB2   | 1.98                     | 0.44              |
| 39:AO:76:ASP:HB2   | 39:AO:109:ARG:HH22 | 1.82                     | 0.44              |
| 69:b:85:ARG:NE     | 69:b:87:GLU:OE2    | 2.44                     | 0.44              |
| 70:c:165:VAL:HG13  | 70:c:222:GLN:HG3   | 2.00                     | 0.44              |
| 1:A:1896:U:C2      | 1:A:1897:A:C8      | 3.06                     | 0.44              |
| 1:A:2072:A:H2'     | 1:A:2073:A:C8      | 2.53                     | 0.44              |
| 1:A:2472:A:N3      | 1:A:2474:C:N4      | 2.66                     | 0.44              |
| 1:A:2514:C:H2'     | 1:A:2515:U:H6      | 1.83                     | 0.44              |
| 6:H:62:VAL:HG11    | 22:X:65:VAL:HG21   | 1.99                     | 0.44              |
| 7:I:188:ARG:O      | 7:I:192:ILE:HG12   | 2.17                     | 0.44              |
| 15:Q:182:ARG:HD2   | 15:Q:218:ASN:HB3   | 1.98                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:AA:1033:U:H4'   | 29:AE:94:VAL:HG12  | 1.99                     | 0.44              |
| 25:AA:1213:A:H1'   | 25:AA:1239:C:O2'   | 2.17                     | 0.44              |
| 26:AB:67:LEU:HD11  | 26:AB:138:ARG:HH21 | 1.82                     | 0.44              |
| 32:AH:76:LEU:HG    | 32:AH:148:LEU:HD11 | 1.99                     | 0.44              |
| 48:AX:93:THR:HG21  | 48:AX:365:TRP:HZ3  | 1.82                     | 0.44              |
| 63:5:103:ALA:HB1   | 63:5:267:GLU:HG3   | 1.99                     | 0.44              |
| 66:8:90:THR:HG23   | 66:8:94:PHE:HD2    | 1.83                     | 0.44              |
| 72:e:187:THR:O     | 72:e:191:THR:HG23  | 2.17                     | 0.44              |
| 80:m:54:VAL:HG11   | 80:m:75:LEU:HG     | 1.98                     | 0.44              |
| 81:o:53:TYR:HD2    | 81:o:54:MET:HG3    | 1.82                     | 0.44              |
| 1:A:1861:U:H2'     | 1:A:1862:U:C6      | 2.53                     | 0.44              |
| 1:A:3158:A:H2'     | 1:A:3159:A:H8      | 1.82                     | 0.44              |
| 4:E:111:THR:OG1    | 4:E:113:ASP:OD1    | 2.28                     | 0.44              |
| 46:AV:138:PHE:CG   | 51:A0:72:PRO:HA    | 2.52                     | 0.44              |
| 64:6:217:LEU:HB3   | 64:6:236:LEU:HD13  | 1.98                     | 0.44              |
| 68:a:46:ASN:O      | 68:a:63:PRO:HD2    | 2.18                     | 0.44              |
| 1:A:2117:U:C2      | 1:A:2118:U:C5      | 3.05                     | 0.44              |
| 6:H:53:THR:OG1     | 22:X:83:GLU:OE2    | 2.29                     | 0.44              |
| 7:I:116:LEU:HB3    | 7:I:121:ILE:HB     | 2.00                     | 0.44              |
| 22:X:125:VAL:HG23  | 22:X:127:VAL:HG13  | 1.99                     | 0.44              |
| 23:Y:104:VAL:HG12  | 67:9:72:PRO:HG3    | 1.98                     | 0.44              |
| 25:AA:1042:U:H2'   | 25:AA:1043:C:C6    | 2.52                     | 0.44              |
| 30:AF:234:ARG:HB2  | 53:A2:53:MET:HE1   | 2.00                     | 0.44              |
| 32:AH:123:SER:HB3  | 32:AH:127:TYR:HB2  | 1.99                     | 0.44              |
| 40:AP:124:TYR:HB3  | 41:AQ:9:ALA:HB2    | 2.00                     | 0.44              |
| 52:A1:137:LEU:HD22 | 52:A1:143:CYS:HA   | 2.00                     | 0.44              |
| 55:A4:308:LYS:HE2  | 55:A4:311:GLU:HG2  | 2.00                     | 0.44              |
| 55:A4:354:LEU:HD11 | 55:A4:388:ARG:HH22 | 1.83                     | 0.44              |
| 56:Ax:8:U:H3       | 56:Ax:14:A:H62     | 1.64                     | 0.44              |
| 59:1:34:ARG:HD3    | 59:1:41:LEU:HG     | 1.99                     | 0.44              |
| 64:6:192:GLU:OE2   | 64:6:322:ARG:NH1   | 2.49                     | 0.44              |
| 66:8:110:GLU:OE2   | 66:8:113:ARG:NH2   | 2.46                     | 0.44              |
| 1:A:1902:C:H1'     | 76:i:126:LYS:HB3   | 1.99                     | 0.44              |
| 1:A:2099:U:H2'     | 1:A:2100:C:H6      | 1.83                     | 0.44              |
| 1:A:2466:A:OP1     | 15:Q:235:ARG:NH1   | 2.49                     | 0.44              |
| 1:A:2495:U:O4      | 1:A:2509:A:H2      | 2.00                     | 0.44              |
| 1:A:2668:A:H2'     | 1:A:2669:A:H8      | 1.82                     | 0.44              |
| 1:A:2693:A:OP1     | 81:o:15:ARG:NH1    | 2.51                     | 0.44              |
| 6:H:62:VAL:HG22    | 6:H:77:HIS:CD2     | 2.51                     | 0.44              |
| 25:AA:942:A:N6     | 25:AA:1047:A:H5'   | 2.32                     | 0.44              |
| 25:AA:1044:U:H2'   | 25:AA:1045:G:O4'   | 2.18                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 28:AD:364:ASP:OD2 | 28:AD:388:ARG:NH1 | 2.50                     | 0.44              |
| 1:A:2166:C:H2'    | 1:A:2167:A:C8     | 2.53                     | 0.44              |
| 5:F:116:THR:O     | 5:F:120:VAL:HG23  | 2.18                     | 0.44              |
| 15:Q:96:ARG:HH21  | 15:Q:286:ILE:HG13 | 1.82                     | 0.44              |
| 25:AA:800:C:H2'   | 25:AA:801:A:C8    | 2.52                     | 0.44              |
| 25:AA:867:C:H2'   | 25:AA:870:C:N4    | 2.33                     | 0.44              |
| 25:AA:1175:G:H2'  | 25:AA:1176:G:H8   | 1.83                     | 0.44              |
| 25:AA:1373:U:H2'  | 25:AA:1374:A:H8   | 1.82                     | 0.44              |
| 48:AX:132:THR:N   | 95:AX:501:ATP:O2B | 2.48                     | 0.44              |
| 64:6:374:GLU:OE2  | 82:p:140:SER:OG   | 2.28                     | 0.44              |
| 72:e:162:ARG:HD2  | 72:e:169:ASP:HB3  | 1.99                     | 0.44              |
| 74:g:96:VAL:HG22  | 74:g:110:ILE:HG12 | 2.00                     | 0.44              |
| 1:A:1894:G:H2'    | 1:A:1895:C:H6     | 1.83                     | 0.44              |
| 1:A:2016:C:H2'    | 1:A:2017:U:H6     | 1.82                     | 0.44              |
| 1:A:2414:C:N4     | 85:s:163:VAL:O    | 2.38                     | 0.44              |
| 1:A:2883:A:H61    | 14:P:172:LEU:HB3  | 1.82                     | 0.44              |
| 8:J:114:LEU:HD12  | 8:J:157:LYS:HG3   | 1.99                     | 0.44              |
| 12:N:105:MET:HG2  | 12:N:179:VAL:HG13 | 2.00                     | 0.44              |
| 16:R:141:ILE:HG22 | 68:a:51:LEU:HD12  | 2.00                     | 0.44              |
| 19:U:8:PRO:HA     | 23:Y:183:GLN:HE22 | 1.83                     | 0.44              |
| 25:AA:881:A:N6    | 39:AO:82:LYS:HB3  | 2.33                     | 0.44              |
| 25:AA:1034:U:H2'  | 25:AA:1035:U:H6   | 1.83                     | 0.44              |
| 25:AA:1035:U:H2'  | 25:AA:1036:A:H8   | 1.82                     | 0.44              |
| 55:A4:80:ARG:HH22 | 55:A4:485:ALA:HB2 | 1.81                     | 0.44              |
| 55:A4:100:SER:OG  | 55:A4:104:ARG:NH1 | 2.51                     | 0.44              |
| 63:5:59:THR:HG22  | 63:5:71:ALA:HB3   | 1.99                     | 0.44              |
| 78:k:11:ARG:HH11  | 78:k:46:ASN:HA    | 1.83                     | 0.44              |
| 80:m:54:VAL:HG21  | 80:m:68:TYR:HB3   | 1.99                     | 0.44              |
| 82:p:82:CYS:O     | 82:p:97:SER:OG    | 2.34                     | 0.44              |
| 83:q:111:GLU:HG3  | 83:q:114:ARG:HH21 | 1.83                     | 0.44              |
| 85:s:119:PRO:HG3  | 85:s:394:TRP:CD2  | 2.53                     | 0.44              |
| 1:A:2728:C:H2'    | 1:A:2729:U:H6     | 1.82                     | 0.43              |
| 1:A:2942:C:H2'    | 1:A:2943:G:H8     | 1.83                     | 0.43              |
| 1:A:3112:A:N7     | 1:A:3200:U:O2     | 2.51                     | 0.43              |
| 3:D:140:ALA:HB2   | 3:D:153:ALA:HB2   | 1.99                     | 0.43              |
| 25:AA:1326:A:O4'  | 28:AD:114:ARG:NH1 | 2.51                     | 0.43              |
| 25:AA:1366:C:H3'  | 25:AA:1367:A:H5'  | 1.99                     | 0.43              |
| 25:AA:1464:G:H2'  | 25:AA:1465:C:C6   | 2.53                     | 0.43              |
| 29:AE:37:ARG:N    | 29:AE:67:ASP:O    | 2.50                     | 0.43              |
| 39:AO:64:TYR:OH   | 39:AO:125:GLN:NE2 | 2.44                     | 0.43              |
| 72:e:159:LEU:HD13 | 72:e:254:TRP:CE2  | 2.53                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 80:m:57:VAL:HG22   | 80:m:63:THR:HG22   | 1.99                     | 0.43              |
| 85:s:113:VAL:HG11  | 85:s:257:VAL:HG21  | 2.00                     | 0.43              |
| 1:A:1993:A:H8      | 1:A:2498:U:HO2'    | 1.66                     | 0.43              |
| 1:A:2011:G:O6      | 76:i:113:ARG:NH1   | 2.40                     | 0.43              |
| 1:A:2346:U:H2'     | 1:A:2347:C:C6      | 2.52                     | 0.43              |
| 1:A:2593:G:O2'     | 1:A:2631:G:O6      | 2.35                     | 0.43              |
| 1:A:2710:C:H2'     | 1:A:2711:A:H8      | 1.83                     | 0.43              |
| 4:E:150:LYS:O      | 4:E:174:GLN:N      | 2.44                     | 0.43              |
| 24:Z:100:HIS:HB3   | 24:Z:106:VAL:HG11  | 2.00                     | 0.43              |
| 26:AB:149:ARG:NH2  | 41:AQ:84:TRP:O     | 2.52                     | 0.43              |
| 31:AG:291:GLY:N    | 31:AG:327:ASP:OD1  | 2.51                     | 0.43              |
| 48:AX:145:CYS:SG   | 48:AX:259:LEU:HD22 | 2.58                     | 0.43              |
| 61:3:154:GLN:O     | 61:3:158:LEU:HG    | 2.19                     | 0.43              |
| 71:d:109:THR:OG1   | 71:d:110:GLU:N     | 2.49                     | 0.43              |
| 83:q:101:GLU:HG3   | 83:q:104:ARG:HH21  | 1.83                     | 0.43              |
| 1:A:1765:C:O3'     | 76:i:75:ARG:NH2    | 2.50                     | 0.43              |
| 1:A:1863:A:H2'     | 1:A:1864:A:C8      | 2.53                     | 0.43              |
| 1:A:2152:A:OP1     | 81:o:34:ASN:HB3    | 2.18                     | 0.43              |
| 18:T:97:LEU:HD22   | 18:T:112:LYS:HG3   | 1.99                     | 0.43              |
| 20:V:137:PHE:HA    | 20:V:143:ARG:HA    | 2.01                     | 0.43              |
| 25:AA:1553:A:H2'   | 25:AA:1554:G:C8    | 2.53                     | 0.43              |
| 27:AC:37:ASN:N     | 27:AC:37:ASN:OD1   | 2.52                     | 0.43              |
| 48:AX:338:ASP:OD1  | 52:A1:312:TYR:OH   | 2.27                     | 0.43              |
| 50:AZ:81:GLU:OE2   | 50:AZ:84:ARG:NH2   | 2.34                     | 0.43              |
| 63:5:218:LEU:HD13  | 63:5:262:ILE:HD13  | 2.00                     | 0.43              |
| 65:7:184:VAL:HG22  | 65:7:294:ILE:HG12  | 1.99                     | 0.43              |
| 70:c:105:ARG:HG3   | 70:c:110:ILE:HB    | 2.00                     | 0.43              |
| 72:e:124:TRP:CE2   | 80:m:72:ARG:HG2    | 2.53                     | 0.43              |
| 72:e:198:ASN:HB2   | 72:e:200:MET:HE2   | 1.99                     | 0.43              |
| 73:f:94:HIS:HB3    | 73:f:156:VAL:HG22  | 2.00                     | 0.43              |
| 1:A:1953:A:OP1     | 4:E:232:GLY:HA2    | 2.19                     | 0.43              |
| 1:A:2164:C:H2'     | 1:A:2165:C:C6      | 2.53                     | 0.43              |
| 1:A:2350:A:H1'     | 1:A:2351:U:H5      | 1.83                     | 0.43              |
| 1:A:2408:U:C2      | 1:A:2409:A:N7      | 2.87                     | 0.43              |
| 2:B:23:A:H2'       | 2:B:24:G:H8        | 1.81                     | 0.43              |
| 12:N:96:TYR:HB3    | 12:N:151:VAL:HB    | 2.00                     | 0.43              |
| 25:AA:856:A:C2     | 25:AA:857:G:C8     | 3.06                     | 0.43              |
| 25:AA:924:A:N3     | 34:AJ:56:PRO:HB3   | 2.34                     | 0.43              |
| 25:AA:1488:5MC:H2' | 25:AA:1489:G:C8    | 2.54                     | 0.43              |
| 27:AC:115:ASN:ND2  | 49:AY:309:LYS:O    | 2.51                     | 0.43              |
| 30:AF:53:LYS:HD2   | 30:AF:58:LEU:HD23  | 1.99                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 65:7:106:ALA:O     | 65:7:113:TRP:N     | 2.52                     | 0.43              |
| 72:e:124:TRP:CD2   | 80:m:72:ARG:HG2    | 2.53                     | 0.43              |
| 78:k:17:ARG:HH12   | 78:k:19:GLN:HB2    | 1.83                     | 0.43              |
| 1:A:2409:A:H2'     | 1:A:2410:U:C6      | 2.54                     | 0.43              |
| 1:A:2465:U:H2'     | 1:A:2466:A:C8      | 2.53                     | 0.43              |
| 1:A:2841:U:OP2     | 21:W:39:SER:OG     | 2.35                     | 0.43              |
| 5:F:92:ARG:HB2     | 5:F:176:VAL:HG21   | 2.00                     | 0.43              |
| 7:I:119:HIS:O      | 7:I:160:LYS:HD2    | 2.19                     | 0.43              |
| 13:O:82:GLU:OE1    | 13:O:82:GLU:N      | 2.52                     | 0.43              |
| 24:Z:69:VAL:HG23   | 24:Z:91:LEU:HD21   | 2.01                     | 0.43              |
| 29:AE:35:ILE:HG13  | 36:AL:97:MET:HE1   | 2.00                     | 0.43              |
| 1:A:2256:U:H2'     | 1:A:2257:C:C6      | 2.54                     | 0.43              |
| 1:A:2508:C:H2'     | 1:A:2509:A:C8      | 2.53                     | 0.43              |
| 19:U:112:PRO:HD2   | 23:Y:75:GLY:HA3    | 1.99                     | 0.43              |
| 25:AA:806:C:C2     | 51:A0:11:ILE:HB    | 2.54                     | 0.43              |
| 25:AA:1173:C:H2'   | 25:AA:1174:U:C6    | 2.54                     | 0.43              |
| 25:AA:1311:C:O2    | 30:AF:36:ARG:NH2   | 2.52                     | 0.43              |
| 26:AB:233:THR:HA   | 43:AS:44:PRO:HG3   | 2.00                     | 0.43              |
| 46:AV:107:TRP:HB3  | 46:AV:382:TRP:CG   | 2.54                     | 0.43              |
| 47:AW:144:LEU:HD23 | 47:AW:167:ALA:HB2  | 2.00                     | 0.43              |
| 48:AX:204:VAL:HG12 | 48:AX:246:GLU:HG3  | 2.00                     | 0.43              |
| 72:e:113:ASP:N     | 72:e:113:ASP:OD1   | 2.50                     | 0.43              |
| 72:e:217:PHE:HE2   | 72:e:226:ASN:HB3   | 1.83                     | 0.43              |
| 1:A:2987:U:O2'     | 1:A:2991:U:OP1     | 2.33                     | 0.43              |
| 6:H:56:VAL:HB      | 6:H:80:TYR:HB3     | 2.00                     | 0.43              |
| 9:K:5:SER:HB2      | 9:K:8:PRO:HD2      | 2.00                     | 0.43              |
| 14:P:178:ILE:HD13  | 82:p:174:LYS:HE2   | 2.00                     | 0.43              |
| 25:AA:1175:G:H2'   | 25:AA:1176:G:C8    | 2.54                     | 0.43              |
| 25:AA:1545:U:H2'   | 25:AA:1546:A:C8    | 2.54                     | 0.43              |
| 28:AD:325:ARG:NH2  | 28:AD:430:THR:OXT  | 2.43                     | 0.43              |
| 36:AL:163:ARG:HD2  | 36:AL:187:ILE:HD13 | 2.00                     | 0.43              |
| 42:AR:194:GLN:NE2  | 42:AR:199:LYS:H    | 2.14                     | 0.43              |
| 46:AV:30:LEU:HD23  | 46:AV:364:LEU:HD21 | 2.00                     | 0.43              |
| 48:AX:205:GLN:HB2  | 48:AX:249:ARG:HH11 | 1.83                     | 0.43              |
| 51:A0:145:HIS:ND1  | 51:A0:146:GLU:HG2  | 2.34                     | 0.43              |
| 66:8:178:TYR:CG    | 80:m:65:HIS:HE1    | 2.37                     | 0.43              |
| 71:d:287:LEU:HD11  | 71:d:293:TYR:HB2   | 2.00                     | 0.43              |
| 73:f:133:GLU:HG2   | 73:f:149:VAL:HG22  | 2.01                     | 0.43              |
| 1:A:1946:C:H2'     | 1:A:1947:C:H6      | 1.83                     | 0.43              |
| 1:A:2186:C:H2'     | 1:A:2187:C:H6      | 1.83                     | 0.43              |
| 1:A:2191:A:N6      | 1:A:2197:G:OP2     | 2.52                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:AA:1292:A:C5   | 31:AG:216:LEU:HD12 | 2.54                     | 0.43              |
| 25:AA:1522:U:O2'  | 46:AV:66:PRO:O     | 2.31                     | 0.43              |
| 27:AC:77:ASP:OD1  | 32:AH:114:LYS:NZ   | 2.36                     | 0.43              |
| 47:AW:149:LEU:HB2 | 47:AW:162:VAL:HG22 | 2.01                     | 0.43              |
| 52:A1:74:ALA:O    | 52:A1:110:ASN:ND2  | 2.42                     | 0.43              |
| 65:7:276:PHE:CD2  | 65:7:277:GLN:HG3   | 2.54                     | 0.43              |
| 72:e:185:ARG:HH21 | 72:e:204:PHE:HB2   | 1.83                     | 0.43              |
| 1:A:2529:U:OP2    | 3:D:208:ARG:HD3    | 2.18                     | 0.43              |
| 5:F:223:HIS:HA    | 5:F:226:MET:HE3    | 2.00                     | 0.43              |
| 19:U:137:ARG:HD2  | 20:V:104:TYR:HE1   | 1.83                     | 0.43              |
| 25:AA:1233:C:O2   | 35:AK:86:ARG:HG2   | 2.18                     | 0.43              |
| 28:AD:317:HIS:CD2 | 28:AD:318:ARG:H    | 2.37                     | 0.43              |
| 43:AS:82:GLN:HE21 | 43:AS:133:ARG:HD3  | 1.82                     | 0.43              |
| 66:8:182:ILE:HB   | 66:8:185:TYR:HB2   | 1.99                     | 0.43              |
| 85:s:332:LEU:HD21 | 85:s:359:ALA:HB2   | 2.00                     | 0.43              |
| 1:A:2841:U:H3'    | 21:W:41:ASN:HD21   | 1.84                     | 0.43              |
| 1:A:3158:A:H2'    | 1:A:3159:A:C8      | 2.54                     | 0.43              |
| 3:D:123:GLU:HG3   | 63:5:258:PRO:HG3   | 2.01                     | 0.43              |
| 3:D:171:ARG:HD3   | 3:D:172:MET:HE2    | 2.01                     | 0.43              |
| 25:AA:1116:A:H2'  | 25:AA:1117:A:C8    | 2.54                     | 0.43              |
| 25:AA:1165:C:H2'  | 25:AA:1166:A:C8    | 2.54                     | 0.43              |
| 25:AA:1452:U:H2'  | 25:AA:1453:A:C8    | 2.53                     | 0.43              |
| 25:AA:1499:U:H2'  | 25:AA:1500:C:H6    | 1.84                     | 0.43              |
| 52:A1:189:LYS:HD3 | 52:A1:233:SER:HA   | 2.01                     | 0.43              |
| 69:b:76:VAL:HG22  | 69:b:86:GLU:HG3    | 2.01                     | 0.43              |
| 84:r:179:PRO:HA   | 84:r:194:LEU:HD13  | 2.01                     | 0.43              |
| 1:A:2081:U:H5''   | 81:o:63:ALA:HB3    | 2.01                     | 0.42              |
| 1:A:2203:G:H2'    | 1:A:2204:U:C6      | 2.54                     | 0.42              |
| 1:A:2747:U:H2'    | 1:A:2748:A:C8      | 2.51                     | 0.42              |
| 20:V:16:PRO:HD2   | 20:V:19:TYR:HB2    | 2.01                     | 0.42              |
| 23:Y:99:HIS:NE2   | 23:Y:103:TYR:HE2   | 2.17                     | 0.42              |
| 24:Z:66:LEU:HD12  | 24:Z:122:LEU:HD23  | 1.99                     | 0.42              |
| 25:AA:845:A:H2'   | 25:AA:846:A:C8     | 2.54                     | 0.42              |
| 25:AA:1033:U:H2'  | 25:AA:1034:U:H6    | 1.84                     | 0.42              |
| 25:AA:1255:U:H2'  | 25:AA:1256:A:C8    | 2.53                     | 0.42              |
| 25:AA:1553:A:H2'  | 25:AA:1554:G:H8    | 1.84                     | 0.42              |
| 35:AK:59:LYS:HB3  | 50:AZ:32:LYS:HD3   | 2.01                     | 0.42              |
| 39:AO:177:PHE:HA  | 42:AR:168:ARG:NE   | 2.34                     | 0.42              |
| 46:AV:275:LEU:O   | 46:AV:348:GLU:N    | 2.40                     | 0.42              |
| 80:m:35:SER:O     | 80:m:39:SER:HB3    | 2.18                     | 0.42              |
| 1:A:2799:U:H2'    | 1:A:2800:U:C6      | 2.54                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:A:2943:G:H2'     | 1:A:2944:C:C6      | 2.54                     | 0.42              |
| 8:J:123:ILE:HG13   | 79:I:75:VAL:HG13   | 2.00                     | 0.42              |
| 12:N:31:LYS:HE3    | 12:N:31:LYS:HB2    | 1.82                     | 0.42              |
| 23:Y:96:GLU:HG2    | 23:Y:100:LYS:HE3   | 2.02                     | 0.42              |
| 25:AA:1067:A:H2'   | 25:AA:1068:A:O4'   | 2.18                     | 0.42              |
| 25:AA:1260:A:C6    | 25:AA:1336:G:C5    | 3.08                     | 0.42              |
| 27:AC:150:PRO:HG3  | 49:AY:309:LYS:HB3  | 2.00                     | 0.42              |
| 43:AS:70:ILE:HB    | 43:AS:100:VAL:HG22 | 2.01                     | 0.42              |
| 53:A2:56:TRP:HE1   | 53:A2:70:ILE:HD11  | 1.84                     | 0.42              |
| 58:0:125:TYR:CZ    | 71:d:289:PRO:HA    | 2.53                     | 0.42              |
| 70:c:192:GLN:HE21  | 70:c:196:PHE:HE2   | 1.68                     | 0.42              |
| 72:e:60:SER:O      | 72:e:136:ARG:NH2   | 2.42                     | 0.42              |
| 72:e:215:PHE:CZ    | 72:e:229:ALA:HB3   | 2.54                     | 0.42              |
| 79:I:107:LEU:HG    | 79:I:117:TYR:CE2   | 2.54                     | 0.42              |
| 81:o:53:TYR:CD2    | 81:o:54:MET:HG3    | 2.55                     | 0.42              |
| 85:s:380:THR:O     | 85:s:384:ASP:HB2   | 2.20                     | 0.42              |
| 1:A:1868:G:H2'     | 11:M:40:PRO:HG3    | 2.00                     | 0.42              |
| 1:A:1989:C:H2'     | 1:A:1990:G:C8      | 2.54                     | 0.42              |
| 1:A:2343:G:N3      | 1:A:2343:G:H3'     | 2.33                     | 0.42              |
| 1:A:2615:A:H1'     | 10:L:81:LYS:HD3    | 2.01                     | 0.42              |
| 1:A:2807:U:H2'     | 1:A:2808:U:C6      | 2.54                     | 0.42              |
| 2:B:68:C:H2'       | 2:B:69:U:C6        | 2.54                     | 0.42              |
| 17:S:163:LYS:HZ2   | 17:S:163:LYS:HB3   | 1.84                     | 0.42              |
| 20:V:64:ILE:HD11   | 20:V:88:VAL:HG21   | 2.00                     | 0.42              |
| 25:AA:1373:U:H2'   | 25:AA:1374:A:C8    | 2.53                     | 0.42              |
| 25:AA:1404:A:C8    | 25:AA:1407:U:C4    | 3.07                     | 0.42              |
| 25:AA:1511:C:OP1   | 51:A0:7:ARG:NH2    | 2.52                     | 0.42              |
| 30:AF:91:ILE:HG23  | 30:AF:111:MET:HE2  | 2.00                     | 0.42              |
| 35:AK:91:CYS:HB3   | 35:AK:96:ARG:H     | 1.84                     | 0.42              |
| 40:AP:95:HIS:CD2   | 40:AP:96:ILE:HG13  | 2.54                     | 0.42              |
| 42:AR:128:MET:SD   | 42:AR:269:GLY:HA3  | 2.59                     | 0.42              |
| 46:AV:79:ILE:HG23  | 46:AV:84:GLU:HB2   | 2.01                     | 0.42              |
| 50:AZ:24:ARG:HG2   | 80:m:110:LEU:HD22  | 2.00                     | 0.42              |
| 55:A4:262:MET:HG3  | 55:A4:266:MET:HE3  | 2.00                     | 0.42              |
| 56:Ax:45:A:H5'     | 56:Ax:46:A:OP2     | 2.19                     | 0.42              |
| 63:5:136:VAL:HG11  | 63:5:417:LEU:HD23  | 2.02                     | 0.42              |
| 80:m:98:ALA:HB1    | 80:m:101:GLN:HE21  | 1.84                     | 0.42              |
| 1:A:2213:A:H3'     | 1:A:2214:A:H5''    | 2.01                     | 0.42              |
| 1:A:3151:A:H4'     | 15:Q:146:GLY:O     | 2.19                     | 0.42              |
| 89:A:6456:G34:H222 | 89:A:6456:G34:H241 | 1.59                     | 0.42              |
| 11:M:68:GLU:OE1    | 11:M:71:GLN:NE2    | 2.53                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:R:101:VAL:HG11 | 17:S:98:VAL:HG11  | 2.02                     | 0.42              |
| 20:V:184:GLU:O    | 23:Y:93:LYS:NZ    | 2.48                     | 0.42              |
| 25:AA:810:G:C2    | 25:AA:811:G:C5    | 3.08                     | 0.42              |
| 25:AA:1057:G:H4'  | 25:AA:1578:A:H4'  | 2.01                     | 0.42              |
| 63:5:125:LYS:HE3  | 63:5:125:LYS:HB3  | 1.88                     | 0.42              |
| 76:i:98:VAL:O     | 76:i:102:MET:HG3  | 2.18                     | 0.42              |
| 1:A:1937:A:H2     | 1:A:1938:A:C5     | 2.38                     | 0.42              |
| 1:A:1939:G:C8     | 3:D:259:LYS:HE3   | 2.55                     | 0.42              |
| 1:A:2482:A:H2'    | 1:A:2483:U:C6     | 2.54                     | 0.42              |
| 1:A:2951:A:H2'    | 1:A:2952:U:C6     | 2.53                     | 0.42              |
| 8:J:90:PHE:HB3    | 8:J:120:ILE:HD13  | 2.01                     | 0.42              |
| 13:O:46:TRP:HD1   | 13:O:121:ALA:HB2  | 1.83                     | 0.42              |
| 25:AA:1359:U:H2'  | 25:AA:1360:G:H8   | 1.84                     | 0.42              |
| 28:AD:317:HIS:HD2 | 28:AD:318:ARG:N   | 2.17                     | 0.42              |
| 42:AR:188:GLU:O   | 42:AR:192:MET:HG2 | 2.20                     | 0.42              |
| 55:A4:356:VAL:O   | 55:A4:360:MET:HG3 | 2.19                     | 0.42              |
| 61:3:152:LYS:HE2  | 61:3:156:LYS:HE3  | 2.01                     | 0.42              |
| 61:3:188:VAL:O    | 64:6:356:ARG:NH2  | 2.41                     | 0.42              |
| 63:5:59:THR:HB    | 63:5:73:PRO:HG3   | 2.01                     | 0.42              |
| 67:9:126:LYS:HB3  | 67:9:126:LYS:HE2  | 1.78                     | 0.42              |
| 72:e:101:LYS:NZ   | 72:e:107:ASP:O    | 2.52                     | 0.42              |
| 77:j:45:GLU:OE2   | 77:j:70:ARG:NH2   | 2.33                     | 0.42              |
| 85:s:100:LEU:HD22 | 85:s:319:GLN:HG3  | 2.00                     | 0.42              |
| 1:A:1898:A:H2'    | 1:A:1899:G:H8     | 1.85                     | 0.42              |
| 1:A:1962:A:OP2    | 1:A:2501:C:N4     | 2.53                     | 0.42              |
| 1:A:2227:A:H2'    | 1:A:2227:A:N3     | 2.35                     | 0.42              |
| 1:A:2698:G:H5''   | 1:A:2699:C:H5     | 1.84                     | 0.42              |
| 1:A:3046:C:H2'    | 1:A:3047:G:C8     | 2.54                     | 0.42              |
| 89:A:6456:G34:H4  | 89:A:6456:G34:H11 | 1.86                     | 0.42              |
| 9:K:36:SER:OG     | 9:K:40:GLN:NE2    | 2.51                     | 0.42              |
| 23:Y:128:SER:HB3  | 23:Y:131:ARG:NE   | 2.35                     | 0.42              |
| 25:AA:1347:G:H2'  | 25:AA:1348:G:H8   | 1.85                     | 0.42              |
| 32:AH:53:ASP:OD1  | 55:A4:436:HIS:NE2 | 2.46                     | 0.42              |
| 34:AJ:72:LYS:HD2  | 57:Az:9:U:H5'     | 2.02                     | 0.42              |
| 46:AV:123:ASP:OD1 | 46:AV:123:ASP:N   | 2.52                     | 0.42              |
| 48:AX:252:SER:O   | 48:AX:302:HIS:NE2 | 2.52                     | 0.42              |
| 55:A4:255:ASN:O   | 55:A4:258:SER:OG  | 2.35                     | 0.42              |
| 72:e:133:LEU:HD22 | 80:m:63:THR:HG21  | 2.01                     | 0.42              |
| 1:A:1840:C:H2'    | 1:A:1841:U:C6     | 2.55                     | 0.42              |
| 1:A:2067:C:H5''   | 73:f:60:LYS:HB2   | 2.01                     | 0.42              |
| 1:A:2982:C:H5''   | 12:N:139:ARG:HG2  | 2.02                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:A:3034:U:H2'     | 1:A:3035:C:C6      | 2.54                     | 0.42              |
| 1:A:3064:A:O4'     | 1:A:3099:C:N4      | 2.52                     | 0.42              |
| 1:A:3143:U:H2'     | 1:A:3144:A:H8      | 1.84                     | 0.42              |
| 25:AA:1354:A:H2'   | 25:AA:1355:G:C8    | 2.54                     | 0.42              |
| 28:AD:160:ARG:NH2  | 28:AD:165:GLN:OE1  | 2.44                     | 0.42              |
| 30:AF:207:HIS:NE2  | 30:AF:211:GLU:OE2  | 2.52                     | 0.42              |
| 36:AL:100:LYS:NZ   | 36:AL:141:GLU:OE1  | 2.47                     | 0.42              |
| 39:AO:208:PRO:HG3  | 45:AU:51:ALA:HA    | 2.01                     | 0.42              |
| 42:AR:209:ILE:HD12 | 42:AR:214:ASN:HB3  | 2.01                     | 0.42              |
| 51:A0:110:ASP:OD1  | 51:A0:110:ASP:N    | 2.47                     | 0.42              |
| 65:7:88:PRO:HB3    | 65:7:125:ILE:HD11  | 2.02                     | 0.42              |
| 72:e:185:ARG:NH1   | 72:e:207:ASN:OD1   | 2.52                     | 0.42              |
| 72:e:272:VAL:HA    | 72:e:275:PHE:CE2   | 2.55                     | 0.42              |
| 84:r:174:MET:N     | 84:r:196:HIS:OXT   | 2.47                     | 0.42              |
| 1:A:2667:U:C2      | 1:A:2668:A:C8      | 3.08                     | 0.42              |
| 4:E:80:LEU:HA      | 4:E:84:PRO:HB3     | 2.00                     | 0.42              |
| 15:Q:74:ARG:HG2    | 15:Q:283:TRP:CZ2   | 2.55                     | 0.42              |
| 20:V:55:TYR:CD1    | 20:V:133:ILE:HD12  | 2.55                     | 0.42              |
| 25:AA:1209:C:H2'   | 25:AA:1210:U:C6    | 2.54                     | 0.42              |
| 25:AA:1427:A:H2'   | 25:AA:1428:G:C8    | 2.55                     | 0.42              |
| 25:AA:1497:C:H2'   | 25:AA:1498:C:C6    | 2.55                     | 0.42              |
| 25:AA:1497:C:H2'   | 25:AA:1498:C:H6    | 1.85                     | 0.42              |
| 26:AB:66:PRO:HB2   | 26:AB:134:HIS:HE1  | 1.85                     | 0.42              |
| 48:AX:203:LYS:O    | 48:AX:250:GLN:NE2  | 2.53                     | 0.42              |
| 51:A0:129:ARG:HH22 | 51:A0:204:PRO:HB2  | 1.84                     | 0.42              |
| 55:A4:302:VAL:HG21 | 55:A4:341:CYS:HB3  | 2.01                     | 0.42              |
| 55:A4:452:GLN:HG2  | 55:A4:453:HIS:CD2  | 2.55                     | 0.42              |
| 65:7:139:ASN:HB3   | 65:7:174:VAL:HG21  | 2.01                     | 0.42              |
| 71:d:94:ASP:OD2    | 71:d:245:TYR:OH    | 2.27                     | 0.42              |
| 71:d:152:LEU:HD22  | 71:d:176:ILE:HD11  | 2.02                     | 0.42              |
| 71:d:226:ASP:OD1   | 71:d:230:ARG:N     | 2.51                     | 0.42              |
| 82:p:84:SER:OG     | 82:p:96:ASN:O      | 2.37                     | 0.42              |
| 1:A:1743:U:H2'     | 1:A:1744:A:H8      | 1.85                     | 0.42              |
| 1:A:1925:A:H2'     | 1:A:1926:A:C8      | 2.54                     | 0.42              |
| 1:A:2006:C:H2'     | 1:A:2007:U:C6      | 2.55                     | 0.42              |
| 1:A:2026:A:H2'     | 1:A:2027:A:C8      | 2.55                     | 0.42              |
| 1:A:2339:G:H21     | 1:A:2427:C:H5'     | 1.85                     | 0.42              |
| 89:A:6456:G34:H4   | 89:A:6456:G34:H131 | 1.83                     | 0.42              |
| 14:P:83:VAL:HG11   | 14:P:158:MET:HE1   | 2.02                     | 0.42              |
| 25:AA:1069:A:H5''  | 25:AA:1070:C:H5    | 1.85                     | 0.42              |
| 30:AF:154:PRO:O    | 30:AF:179:ARG:HD2  | 2.20                     | 0.42              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 46:AV:323:GLU:OE1  | 46:AV:330:TYR:OH  | 2.30                     | 0.42              |
| 51:A0:143:PRO:O    | 51:A0:147:GLU:HG3 | 2.20                     | 0.42              |
| 65:7:192:TRP:CD1   | 68:a:91:VAL:HG21  | 2.54                     | 0.42              |
| 1:A:2408:U:H2'     | 1:A:2409:A:C8     | 2.51                     | 0.42              |
| 1:A:2635:G:H2'     | 1:A:2636:G:H8     | 1.85                     | 0.42              |
| 1:A:2724:G:H2'     | 1:A:2988:C:O2'    | 2.20                     | 0.42              |
| 1:A:3024:U:H2'     | 1:A:3025:A:C8     | 2.54                     | 0.42              |
| 25:AA:871:A:O4'    | 25:AA:919:A:N6    | 2.53                     | 0.42              |
| 25:AA:990:U:H2'    | 25:AA:991:G:O4'   | 2.20                     | 0.42              |
| 25:AA:1203:C:H2'   | 25:AA:1204:C:H6   | 1.84                     | 0.42              |
| 25:AA:1255:U:O2'   | 25:AA:1256:A:OP1  | 2.34                     | 0.42              |
| 33:AI:92:HIS:HA    | 33:AI:156:PRO:HD2 | 2.02                     | 0.42              |
| 37:AM:38:HIS:HB2   | 37:AM:41:CYS:SG   | 2.60                     | 0.42              |
| 46:AV:205:GLY:HA2  | 46:AV:227:GLY:HA2 | 2.01                     | 0.42              |
| 55:A4:170:VAL:HG21 | 55:A4:243:ASN:HB3 | 2.02                     | 0.42              |
| 85:s:152:GLN:OE1   | 85:s:179:GLN:NE2  | 2.43                     | 0.42              |
| 1:A:1799:U:H2'     | 1:A:1800:G:O4'    | 2.20                     | 0.41              |
| 1:A:2366:G:H2'     | 1:A:2367:A:C8     | 2.55                     | 0.41              |
| 1:A:2407:U:H2'     | 1:A:2408:U:C6     | 2.53                     | 0.41              |
| 9:K:27:PRO:HG2     | 9:K:30:LYS:HD2    | 2.02                     | 0.41              |
| 9:K:34:MET:O       | 9:K:38:ARG:HG2    | 2.20                     | 0.41              |
| 14:P:167:GLU:O     | 82:p:187:ARG:NH1  | 2.35                     | 0.41              |
| 17:S:163:LYS:HB2   | 69:b:106:ASP:HB3  | 2.02                     | 0.41              |
| 22:X:72:PRO:HB2    | 22:X:74:GLU:HG2   | 2.02                     | 0.41              |
| 25:AA:1495:C:H2'   | 25:AA:1496:U:C6   | 2.55                     | 0.41              |
| 30:AF:149:LEU:O    | 30:AF:153:GLU:HG3 | 2.19                     | 0.41              |
| 38:AN:6:SER:OG     | 38:AN:69:LEU:O    | 2.35                     | 0.41              |
| 55:A4:160:ARG:NH1  | 55:A4:172:MET:SD  | 2.93                     | 0.41              |
| 55:A4:335:PHE:CD2  | 55:A4:360:MET:HG2 | 2.54                     | 0.41              |
| 63:5:132:LEU:HD21  | 63:5:354:PHE:HB2  | 2.01                     | 0.41              |
| 73:f:88:TYR:HE2    | 73:f:164:ALA:HA   | 1.84                     | 0.41              |
| 82:p:113:GLU:OE1   | 82:p:116:ARG:NH2  | 2.33                     | 0.41              |
| 1:A:2035:U:O2'     | 11:M:70:GLY:HA3   | 2.20                     | 0.41              |
| 1:A:2355:A:H2'     | 1:A:2356:A:O4'    | 2.19                     | 0.41              |
| 1:A:2675:G:OP1     | 18:T:163:LYS:HA   | 2.20                     | 0.41              |
| 1:A:2677:A:H2'     | 1:A:2678:A:H8     | 1.82                     | 0.41              |
| 1:A:2795:U:C2      | 1:A:2796:G:C8     | 3.08                     | 0.41              |
| 2:B:63:G:H2'       | 2:B:64:A:H8       | 1.85                     | 0.41              |
| 3:D:141:LEU:HD11   | 3:D:148:LYS:HG2   | 2.02                     | 0.41              |
| 5:F:280:TYR:N      | 74:g:55:THR:O     | 2.45                     | 0.41              |
| 7:I:79:ILE:HG23    | 7:I:130:VAL:HG22  | 2.02                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 10:L:123:ILE:HD12  | 10:L:127:LEU:HD12  | 2.02                     | 0.41              |
| 10:L:128:ARG:HB2   | 15:Q:125:TYR:HB3   | 2.01                     | 0.41              |
| 16:R:149:HIS:ND1   | 24:Z:152:LYS:O     | 2.53                     | 0.41              |
| 25:AA:683:G:H5''   | 44:AT:160:ARG:NH2  | 2.35                     | 0.41              |
| 25:AA:861:U:H2'    | 25:AA:862:A:H8     | 1.85                     | 0.41              |
| 28:AD:281:TYR:CG   | 43:AS:18:ASP:HB3   | 2.55                     | 0.41              |
| 44:AT:80:LEU:HD12  | 44:AT:84:GLU:HB3   | 2.01                     | 0.41              |
| 48:AX:206:GLU:HA   | 48:AX:218:LYS:HE2  | 2.03                     | 0.41              |
| 58:0:166:SER:O     | 58:0:170:GLN:HG3   | 2.20                     | 0.41              |
| 64:6:364:ARG:O     | 64:6:368:ARG:HG3   | 2.20                     | 0.41              |
| 66:8:165:ASP:HB3   | 66:8:168:LEU:HB2   | 2.02                     | 0.41              |
| 71:d:137:PHE:N     | 71:d:138:PRO:HD2   | 2.36                     | 0.41              |
| 1:A:1893:A:H1'     | 1:A:1894:G:C8      | 2.55                     | 0.41              |
| 2:B:4:A:H2'        | 2:B:5:G:C8         | 2.55                     | 0.41              |
| 90:B:101:VAL:HB    | 72:e:165:PHE:HB3   | 2.01                     | 0.41              |
| 11:M:53:HIS:CG     | 11:M:54:LYS:H      | 2.37                     | 0.41              |
| 12:N:191:SER:H     | 12:N:194:THR:HG1   | 1.63                     | 0.41              |
| 22:X:125:VAL:HG12  | 63:5:48:ARG:NH1    | 2.34                     | 0.41              |
| 42:AR:325:ILE:HG22 | 42:AR:329:LYS:HE2  | 2.02                     | 0.41              |
| 44:AT:104:LYS:HD3  | 45:AU:108:TRP:CH2  | 2.55                     | 0.41              |
| 46:AV:190:LEU:HD23 | 46:AV:196:PHE:CZ   | 2.55                     | 0.41              |
| 48:AX:205:GLN:HB2  | 48:AX:249:ARG:NH1  | 2.35                     | 0.41              |
| 63:5:236:LEU:HD21  | 63:5:289:HIS:CD2   | 2.56                     | 0.41              |
| 65:7:97:GLU:O      | 65:7:101:ARG:HG2   | 2.21                     | 0.41              |
| 70:c:170:ALA:HB1   | 70:c:175:VAL:HB    | 2.02                     | 0.41              |
| 85:s:75:SER:HB2    | 85:s:78:GLU:HG3    | 2.01                     | 0.41              |
| 1:A:1860:A:H2'     | 1:A:1861:U:C6      | 2.55                     | 0.41              |
| 1:A:2087:U:H2'     | 1:A:2088:U:C6      | 2.55                     | 0.41              |
| 3:D:74:ILE:HB      | 3:D:150:TRP:HE1    | 1.86                     | 0.41              |
| 25:AA:1034:U:H2'   | 25:AA:1035:U:C6    | 2.56                     | 0.41              |
| 25:AA:1118:A:N1    | 28:AD:297:ARG:NH1  | 2.69                     | 0.41              |
| 27:AC:89:ASP:OD1   | 27:AC:112:ARG:NH2  | 2.45                     | 0.41              |
| 28:AD:289:THR:HG21 | 28:AD:308:GLN:O    | 2.20                     | 0.41              |
| 30:AF:52:ARG:NH2   | 31:AG:319:PHE:O    | 2.53                     | 0.41              |
| 30:AF:88:ASP:HB3   | 30:AF:91:ILE:HB    | 2.02                     | 0.41              |
| 48:AX:159:HIS:O    | 48:AX:163:LYS:HG2  | 2.20                     | 0.41              |
| 52:A1:176:LYS:HG2  | 52:A1:204:VAL:HG22 | 2.03                     | 0.41              |
| 52:A1:181:ASN:O    | 52:A1:234:TRP:NE1  | 2.46                     | 0.41              |
| 65:7:204:LYS:HD3   | 68:a:99:LYS:HZ3    | 1.85                     | 0.41              |
| 69:b:103:LYS:O     | 69:b:107:GLN:HG3   | 2.20                     | 0.41              |
| 70:c:69:HIS:HE1    | 70:c:85:LEU:HD13   | 1.86                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 72:e:88:GLU:OE2    | 80:m:50:ARG:NH1    | 2.42                     | 0.41              |
| 78:k:41:LYS:O      | 78:k:45:THR:HG23   | 2.20                     | 0.41              |
| 1:A:1993:A:H8      | 1:A:2498:U:O2'     | 2.04                     | 0.41              |
| 1:A:2650:C:H2'     | 1:A:2651:A:C8      | 2.55                     | 0.41              |
| 1:A:2815:OMG:OP1   | 12:N:139:ARG:NH1   | 2.54                     | 0.41              |
| 1:A:2832:A:N1      | 64:6:27:ARG:N      | 2.69                     | 0.41              |
| 1:A:2930:U:H2'     | 1:A:2931:A:C8      | 2.55                     | 0.41              |
| 3:D:210:ALA:HB1    | 3:D:249:ASN:HB2    | 2.03                     | 0.41              |
| 7:I:76:ILE:HG22    | 7:I:78:LEU:N       | 2.35                     | 0.41              |
| 15:Q:165:GLU:HB2   | 15:Q:168:ASN:HB2   | 2.03                     | 0.41              |
| 23:Y:163:ALA:HB1   | 67:9:133:ARG:HB2   | 2.03                     | 0.41              |
| 25:AA:776:A:O3'    | 25:AA:777:G:H8     | 2.03                     | 0.41              |
| 25:AA:1133:C:H2'   | 25:AA:1134:G:H8    | 1.85                     | 0.41              |
| 25:AA:1203:C:H2'   | 25:AA:1204:C:C6    | 2.54                     | 0.41              |
| 25:AA:1439:A:H2'   | 25:AA:1440:G:C8    | 2.55                     | 0.41              |
| 31:AG:69:TYR:H     | 31:AG:135:GLN:HE22 | 1.68                     | 0.41              |
| 51:A0:64:LEU:HB2   | 51:A0:139:TRP:CD2  | 2.56                     | 0.41              |
| 55:A4:482:ILE:HA   | 55:A4:483:PRO:HA   | 1.95                     | 0.41              |
| 65:7:103:SER:HA    | 65:7:129:THR:HG22  | 2.01                     | 0.41              |
| 1:A:2010:U:O4'     | 1:A:2012:A:H5'     | 2.21                     | 0.41              |
| 1:A:2175:C:O2'     | 8:J:102:ARG:NH2    | 2.53                     | 0.41              |
| 1:A:2212:C:H2'     | 1:A:2213:A:H8      | 1.85                     | 0.41              |
| 1:A:2734:A:H2'     | 1:A:2735:G:C8      | 2.55                     | 0.41              |
| 1:A:2951:A:H2'     | 1:A:2952:U:H6      | 1.86                     | 0.41              |
| 12:N:117:ASN:OD1   | 12:N:166:ARG:NH2   | 2.54                     | 0.41              |
| 20:V:105:ARG:H     | 20:V:105:ARG:HG2   | 1.69                     | 0.41              |
| 25:AA:1138:G:H2'   | 25:AA:1139:A:H8    | 1.84                     | 0.41              |
| 25:AA:1191:C:H2'   | 25:AA:1192:C:C6    | 2.56                     | 0.41              |
| 26:AB:169:ARG:NH1  | 41:AQ:87:CYS:HA    | 2.36                     | 0.41              |
| 28:AD:294:ILE:HD11 | 28:AD:356:GLN:HB3  | 2.02                     | 0.41              |
| 35:AK:120:LEU:HB3  | 35:AK:123:ILE:HD12 | 2.02                     | 0.41              |
| 40:AP:103:LYS:HD3  | 40:AP:103:LYS:HA   | 1.86                     | 0.41              |
| 42:AR:132:LEU:HD12 | 42:AR:237:PRO:HB2  | 2.02                     | 0.41              |
| 55:A4:384:ASP:HB2  | 55:A4:385:PRO:HD3  | 2.02                     | 0.41              |
| 62:4:69:LYS:HB2    | 62:4:72:LEU:HD23   | 2.02                     | 0.41              |
| 67:9:43:PHE:HE1    | 67:9:53:ILE:HD11   | 1.86                     | 0.41              |
| 82:p:76:ARG:NH1    | 82:p:109:GLU:OE1   | 2.50                     | 0.41              |
| 82:p:115:VAL:HG13  | 82:p:161:ALA:HB3   | 2.02                     | 0.41              |
| 84:r:78:LYS:HG2    | 84:r:79:HIS:CD2    | 2.55                     | 0.41              |
| 1:A:2098:G:HO2'    | 1:A:2099:U:H6      | 1.66                     | 0.41              |
| 1:A:2347:C:H2'     | 1:A:2348:A:C8      | 2.55                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:A:2552:U:H2'     | 1:A:2553:G:H8      | 1.86                     | 0.41              |
| 1:A:2943:G:H2'     | 1:A:2944:C:H6      | 1.86                     | 0.41              |
| 1:A:3224:G:H2'     | 1:A:3225:G:H8      | 1.86                     | 0.41              |
| 15:Q:77:SER:HB3    | 15:Q:80:PHE:HD2    | 1.85                     | 0.41              |
| 19:U:114:LYS:H     | 19:U:114:LYS:HG3   | 1.69                     | 0.41              |
| 20:V:121:LYS:HD3   | 20:V:130:PRO:HB2   | 2.03                     | 0.41              |
| 20:V:194:LEU:HA    | 23:Y:95:ASN:HD22   | 1.86                     | 0.41              |
| 25:AA:663:A:H2'    | 25:AA:664:G:H8     | 1.86                     | 0.41              |
| 25:AA:821:U:H2'    | 25:AA:822:G:C8     | 2.48                     | 0.41              |
| 25:AA:1504:U:H2'   | 25:AA:1505:A:H8    | 1.85                     | 0.41              |
| 29:AE:35:ILE:HD11  | 36:AL:91:ARG:HD3   | 2.02                     | 0.41              |
| 30:AF:159:VAL:HG23 | 30:AF:172:VAL:HG21 | 2.02                     | 0.41              |
| 48:AX:192:LYS:HB2  | 48:AX:226:VAL:HG11 | 2.02                     | 0.41              |
| 61:3:96:TYR:OH     | 76:i:128:ARG:O     | 2.31                     | 0.41              |
| 1:A:1851:G:H2'     | 1:A:2693:A:N7      | 2.36                     | 0.41              |
| 1:A:1894:G:H2'     | 1:A:1895:C:C6      | 2.55                     | 0.41              |
| 1:A:1942:C:H2'     | 1:A:1943:A:O4'     | 2.20                     | 0.41              |
| 1:A:2172:A:OP2     | 8:J:21:ARG:NH2     | 2.54                     | 0.41              |
| 1:A:2181:A:C4      | 1:A:2207:A:H4'     | 2.56                     | 0.41              |
| 1:A:2814:G:O2'     | 1:A:2983:G:OP1     | 2.34                     | 0.41              |
| 1:A:2971:A:O2'     | 12:N:182:LYS:O     | 2.37                     | 0.41              |
| 2:B:27:C:H4'       | 66:8:133:ARG:HH22  | 1.86                     | 0.41              |
| 5:F:65:TRP:CD1     | 75:h:117:LEU:HD11  | 2.56                     | 0.41              |
| 7:I:166:ARG:O      | 7:I:170:THR:HG23   | 2.20                     | 0.41              |
| 9:K:138:LEU:HD11   | 69:b:146:ARG:HB2   | 2.02                     | 0.41              |
| 11:M:203:ARG:NH2   | 11:M:261:ASP:O     | 2.53                     | 0.41              |
| 20:V:87:VAL:HG22   | 20:V:114:PRO:HA    | 2.01                     | 0.41              |
| 23:Y:160:GLN:HG3   | 67:9:131:TYR:CD2   | 2.56                     | 0.41              |
| 25:AA:1255:U:H2'   | 25:AA:1256:A:H8    | 1.85                     | 0.41              |
| 25:AA:1408:A:H2'   | 25:AA:1409:A:C8    | 2.55                     | 0.41              |
| 27:AC:98:GLY:HA3   | 50:AZ:71:TYR:CE1   | 2.56                     | 0.41              |
| 28:AD:289:THR:HG22 | 28:AD:331:ASP:O    | 2.21                     | 0.41              |
| 39:AO:148:LYS:HE3  | 39:AO:148:LYS:HB2  | 1.85                     | 0.41              |
| 41:AQ:72:ILE:HG23  | 53:A2:104:LEU:HD11 | 2.02                     | 0.41              |
| 56:Ax:54:U:H2'     | 56:Ax:55:U:O4'     | 2.21                     | 0.41              |
| 66:8:193:ASN:O     | 73:f:133:GLU:N     | 2.44                     | 0.41              |
| 70:c:269:LEU:HD21  | 70:c:271:PHE:HE1   | 1.86                     | 0.41              |
| 71:d:153:ASN:HD21  | 71:d:183:TRP:H     | 1.69                     | 0.41              |
| 77:j:112:LYS:HA    | 77:j:116:LEU:HA    | 2.02                     | 0.41              |
| 85:s:201:ASP:HB2   | 85:s:240:GLN:HG2   | 2.03                     | 0.41              |
| 1:A:1928:A:H2'     | 1:A:1929:A:C8      | 2.55                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:2155:A:N6     | 84:r:169:TRP:O    | 2.54                     | 0.41              |
| 1:A:2158:U:OP2    | 84:r:195:TYR:OH   | 2.27                     | 0.41              |
| 1:A:2177:U:N3     | 1:A:2180:A:OP2    | 2.32                     | 0.41              |
| 1:A:2321:A:C2     | 58:0:142:GLY:HA3  | 2.55                     | 0.41              |
| 1:A:2410:U:H2'    | 1:A:2411:U:H6     | 1.86                     | 0.41              |
| 1:A:2414:C:N3     | 85:s:164:HIS:HA   | 2.35                     | 0.41              |
| 1:A:2417:C:H2'    | 85:s:310:ARG:HH21 | 1.86                     | 0.41              |
| 1:A:2481:A:H2'    | 1:A:2482:A:H8     | 1.85                     | 0.41              |
| 1:A:2552:U:C2     | 1:A:2553:G:C8     | 3.09                     | 0.41              |
| 1:A:2664:U:H2'    | 1:A:2665:U:H6     | 1.86                     | 0.41              |
| 1:A:3014:G:H5''   | 62:4:96:PRO:HB2   | 2.03                     | 0.41              |
| 1:A:3102:U:C2     | 58:0:81:PRO:HA    | 2.56                     | 0.41              |
| 1:A:3202:U:H2'    | 1:A:3203:A:H8     | 1.86                     | 0.41              |
| 4:E:64:LEU:HD23   | 4:E:64:LEU:HA     | 1.90                     | 0.41              |
| 15:Q:89:PRO:HA    | 15:Q:92:PHE:HD2   | 1.86                     | 0.41              |
| 15:Q:95:GLU:OE2   | 15:Q:145:LEU:N    | 2.53                     | 0.41              |
| 15:Q:148:THR:HG22 | 15:Q:165:GLU:HG2  | 2.03                     | 0.41              |
| 23:Y:71:PRO:HA    | 23:Y:74:TRP:CD2   | 2.56                     | 0.41              |
| 25:AA:1181:G:H2'  | 25:AA:1182:C:C6   | 2.56                     | 0.41              |
| 25:AA:1358:A:O2'  | 56:Ax:30:G:OP1    | 2.39                     | 0.41              |
| 25:AA:1407:U:H2'  | 25:AA:1408:A:C8   | 2.55                     | 0.41              |
| 25:AA:1586:G:H2'  | 25:AA:1587:U:C6   | 2.56                     | 0.41              |
| 27:AC:95:PHE:HD1  | 50:AZ:62:MET:HE1  | 1.86                     | 0.41              |
| 29:AE:63:TYR:OH   | 40:AP:118:GLY:O   | 2.27                     | 0.41              |
| 40:AP:141:ARG:HA  | 41:AQ:28:ARG:HH21 | 1.86                     | 0.41              |
| 42:AR:79:LEU:HD22 | 42:AR:269:GLY:HA2 | 2.02                     | 0.41              |
| 46:AV:198:TRP:NE1 | 46:AV:199:GLU:OE2 | 2.53                     | 0.41              |
| 46:AV:393:GLU:OE2 | 46:AV:397:ARG:NE  | 2.46                     | 0.41              |
| 48:AX:162:VAL:O   | 48:AX:272:THR:OG1 | 2.28                     | 0.41              |
| 48:AX:208:TYR:O   | 48:AX:216:THR:N   | 2.54                     | 0.41              |
| 56:Ax:39:C:C2     | 56:Ax:40:C:C5     | 3.09                     | 0.41              |
| 56:Ax:70:A:H2'    | 56:Ax:71:C:C6     | 2.56                     | 0.41              |
| 58:0:152:PRO:HG3  | 58:0:173:ARG:CZ   | 2.51                     | 0.41              |
| 1:A:1679:U:H2'    | 1:A:1680:A:C8     | 2.56                     | 0.41              |
| 1:A:1952:U:H2'    | 1:A:1953:A:C8     | 2.56                     | 0.41              |
| 1:A:2026:A:H2'    | 1:A:2027:A:H8     | 1.86                     | 0.41              |
| 1:A:2161:A:O2'    | 1:A:2162:C:O5'    | 2.33                     | 0.41              |
| 1:A:2186:C:H2'    | 1:A:2187:C:C6     | 2.56                     | 0.41              |
| 1:A:2285:U:H5''   | 70:c:36:ARG:HH12  | 1.86                     | 0.41              |
| 1:A:2802:A:H2'    | 1:A:2803:A:O4'    | 2.20                     | 0.41              |
| 1:A:2996:G:C2     | 1:A:2997:A:C8     | 3.09                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 5:F:217:LEU:HB2   | 5:F:256:HIS:CG     | 2.56                     | 0.41              |
| 5:F:257:GLN:HG2   | 11:M:21:ARG:CZ     | 2.50                     | 0.41              |
| 11:M:295:THR:HG22 | 82:p:39:PHE:HE1    | 1.85                     | 0.41              |
| 25:AA:1130:G:H2'  | 25:AA:1131:C:C6    | 2.55                     | 0.41              |
| 25:AA:1182:C:H2'  | 25:AA:1183:U:C6    | 2.55                     | 0.41              |
| 25:AA:1396:C:H2'  | 25:AA:1397:U:H6    | 1.86                     | 0.41              |
| 27:AC:69:LEU:HD23 | 52:A1:107:LYS:HD3  | 2.01                     | 0.41              |
| 31:AG:318:HIS:NE2 | 48:AX:379:GLU:OE2  | 2.54                     | 0.41              |
| 37:AM:67:ALA:HB2  | 42:AR:196:TYR:CZ   | 2.56                     | 0.41              |
| 41:AQ:77:ARG:HG2  | 41:AQ:80:ARG:HH12  | 1.86                     | 0.41              |
| 56:Ax:51:U:H2'    | 56:Ax:52:G:C8      | 2.55                     | 0.41              |
| 69:b:15:LEU:HD11  | 70:c:169:VAL:HA    | 2.02                     | 0.41              |
| 70:c:83:PHE:CE2   | 70:c:202:LEU:HB2   | 2.55                     | 0.41              |
| 70:c:168:HIS:CE1  | 70:c:172:ASN:HD21  | 2.39                     | 0.41              |
| 70:c:285:PRO:HD2  | 70:c:295:GLU:HG2   | 2.03                     | 0.41              |
| 74:g:138:THR:HG22 | 74:g:149:ILE:HG12  | 2.01                     | 0.41              |
| 77:j:102:GLN:O    | 77:j:106:GLU:HG3   | 2.21                     | 0.41              |
| 1:A:3176:A:H62    | 1:A:3187:C:H1'     | 1.85                     | 0.40              |
| 5:F:61:PRO:HA     | 5:F:84:PRO:HD3     | 2.03                     | 0.40              |
| 13:O:148:LEU:HD22 | 65:7:177:GLY:HA2   | 2.02                     | 0.40              |
| 18:T:151:ARG:HB2  | 18:T:161:MET:HE3   | 2.03                     | 0.40              |
| 25:AA:722:C:H5'   | 51:A0:4:LYS:NZ     | 2.36                     | 0.40              |
| 25:AA:871:A:H1'   | 25:AA:872:G:C8     | 2.56                     | 0.40              |
| 25:AA:952:A:H2'   | 25:AA:953:U:C6     | 2.56                     | 0.40              |
| 25:AA:1033:U:H2'  | 25:AA:1034:U:C6    | 2.56                     | 0.40              |
| 25:AA:1151:C:H5'  | 25:AA:1152:A:N7    | 2.36                     | 0.40              |
| 25:AA:1221:A:OP2  | 25:AA:1222:A:O2'   | 2.27                     | 0.40              |
| 25:AA:1231:A:OP1  | 35:AK:88:ARG:NH2   | 2.52                     | 0.40              |
| 25:AA:1436:C:H2'  | 25:AA:1437:U:C6    | 2.57                     | 0.40              |
| 25:AA:1581:G:H2'  | 25:AA:1583:MA6:OP2 | 2.21                     | 0.40              |
| 26:AB:61:LYS:HD2  | 26:AB:271:TYR:HE1  | 1.85                     | 0.40              |
| 31:AG:110:TYR:OH  | 52:A1:114:LEU:O    | 2.27                     | 0.40              |
| 35:AK:88:ARG:HH21 | 35:AK:98:ARG:HG3   | 1.86                     | 0.40              |
| 38:AN:17:VAL:HG22 | 38:AN:28:VAL:HG22  | 2.03                     | 0.40              |
| 51:A0:83:LYS:N    | 51:A0:138:ASP:OD1  | 2.50                     | 0.40              |
| 65:7:276:PHE:HB2  | 65:7:304:VAL:HG22  | 2.03                     | 0.40              |
| 85:s:63:ILE:HA    | 85:s:66:TRP:HD1    | 1.81                     | 0.40              |
| 1:A:2873:A:H4'    | 21:W:90:TYR:CZ     | 2.56                     | 0.40              |
| 1:A:3114:U:H2'    | 1:A:3115:U:C6      | 2.56                     | 0.40              |
| 1:A:3124:U:H2'    | 1:A:3125:A:H8      | 1.85                     | 0.40              |
| 1:A:3189:C:OP2    | 84:r:158:SER:HB3   | 2.21                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:D:198:SER:HB2    | 3:D:206:TYR:CE2    | 2.56                     | 0.40              |
| 4:E:96:ARG:HD2     | 4:E:197:HIS:CE1    | 2.56                     | 0.40              |
| 4:E:222:TRP:CD1    | 4:E:256:LYS:HB3    | 2.57                     | 0.40              |
| 14:P:60:SER:HB3    | 82:p:177:ARG:HH11  | 1.86                     | 0.40              |
| 22:X:30:ARG:O      | 22:X:34:GLU:HG3    | 2.21                     | 0.40              |
| 25:AA:1470:A:C2    | 25:AA:1471:A:C5    | 3.09                     | 0.40              |
| 28:AD:305:MET:HG2  | 28:AD:334:ALA:HB2  | 2.04                     | 0.40              |
| 31:AG:136:ARG:HB3  | 31:AG:210:VAL:HG11 | 2.03                     | 0.40              |
| 31:AG:206:GLU:OE1  | 31:AG:213:LEU:N    | 2.54                     | 0.40              |
| 35:AK:43:MET:SD    | 35:AK:81:ASP:HB2   | 2.61                     | 0.40              |
| 52:A1:166:PRO:O    | 52:A1:169:ARG:NH1  | 2.53                     | 0.40              |
| 55:A4:414:LYS:HG2  | 55:A4:453:HIS:HE1  | 1.85                     | 0.40              |
| 58:0:137:ILE:HD13  | 58:0:158:VAL:HG21  | 2.04                     | 0.40              |
| 70:c:270:TYR:O     | 70:c:285:PRO:HA    | 2.21                     | 0.40              |
| 1:A:1861:U:H2'     | 1:A:1862:U:H6      | 1.87                     | 0.40              |
| 1:A:2149:G:OP1     | 77:j:23:ALA:N      | 2.54                     | 0.40              |
| 1:A:2815:OMG:HM23  | 1:A:2815:OMG:H1'   | 1.86                     | 0.40              |
| 9:K:118:ARG:O      | 9:K:122:MET:HG2    | 2.21                     | 0.40              |
| 9:K:169:LEU:HD22   | 84:r:75:TRP:CG     | 2.56                     | 0.40              |
| 15:Q:210:GLU:HB2   | 15:Q:213:GLN:HG3   | 2.02                     | 0.40              |
| 17:S:113:LEU:HB2   | 69:b:120:HIS:HB3   | 2.04                     | 0.40              |
| 20:V:96:ARG:HE     | 20:V:111:SER:HB2   | 1.86                     | 0.40              |
| 25:AA:870:C:H5''   | 39:AO:97:ARG:NH1   | 2.36                     | 0.40              |
| 44:AT:52:ILE:HD13  | 44:AT:52:ILE:HA    | 1.97                     | 0.40              |
| 63:5:189:LYS:O     | 63:5:192:ILE:HG13  | 2.22                     | 0.40              |
| 65:7:234:LYS:HA    | 65:7:237:VAL:HG22  | 2.03                     | 0.40              |
| 70:c:44:GLU:HA     | 70:c:47:ARG:HD3    | 2.03                     | 0.40              |
| 1:A:1964:U:H2'     | 1:A:1965:A:C8      | 2.57                     | 0.40              |
| 1:A:2239:A:H2'     | 1:A:2240:C:C6      | 2.57                     | 0.40              |
| 1:A:2439:U:H2'     | 1:A:2440:G:H8      | 1.86                     | 0.40              |
| 1:A:2678:A:H2      | 58:0:80:ALA:HA     | 1.86                     | 0.40              |
| 2:B:27:C:H2'       | 2:B:28:C:H6        | 1.86                     | 0.40              |
| 4:E:219:MET:HE2    | 4:E:219:MET:HB3    | 1.99                     | 0.40              |
| 20:V:181:ASP:O     | 23:Y:93:LYS:NZ     | 2.49                     | 0.40              |
| 22:X:12:LYS:HA     | 22:X:12:LYS:HD3    | 1.89                     | 0.40              |
| 25:AA:968:U:H2'    | 25:AA:969:A:H8     | 1.87                     | 0.40              |
| 25:AA:1279:C:H2'   | 25:AA:1280:C:H6    | 1.85                     | 0.40              |
| 25:AA:1523:A:N7    | 46:AV:396:GLN:NE2  | 2.55                     | 0.40              |
| 26:AB:220:VAL:HG22 | 26:AB:234:TYR:HB2  | 2.04                     | 0.40              |
| 28:AD:282:ILE:HG23 | 28:AD:353:LEU:HB3  | 2.03                     | 0.40              |
| 36:AL:171:ARG:HG3  | 36:AL:175:TYR:HD1  | 1.86                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 37:AM:108:GLU:OE2  | 45:AU:59:ARG:NH2   | 2.33                     | 0.40              |
| 48:AX:136:LEU:HD23 | 48:AX:136:LEU:HA   | 1.92                     | 0.40              |
| 48:AX:244:LEU:HD12 | 48:AX:292:ASN:HB3  | 2.02                     | 0.40              |
| 52:A1:152:ASP:HB2  | 52:A1:172:VAL:HB   | 2.04                     | 0.40              |
| 55:A4:596:LEU:HD21 | 55:A4:614:LEU:HD13 | 2.03                     | 0.40              |
| 63:5:201:ARG:NH1   | 63:5:418:TYR:O     | 2.39                     | 0.40              |
| 65:7:180:CYS:HB2   | 65:7:296:ARG:HG3   | 2.04                     | 0.40              |
| 1:A:1946:C:H2'     | 1:A:1947:C:C6      | 2.55                     | 0.40              |
| 1:A:2339:G:H4'     | 60:2:55:PRO:HB2    | 2.02                     | 0.40              |
| 1:A:2408:U:O2      | 1:A:2409:A:C8      | 2.74                     | 0.40              |
| 1:A:2664:U:H2'     | 1:A:2665:U:C6      | 2.57                     | 0.40              |
| 90:B:101:VAL:O     | 72:e:218:PRO:HD3   | 2.21                     | 0.40              |
| 10:L:125:THR:HG22  | 10:L:144:PHE:HB3   | 2.03                     | 0.40              |
| 14:P:72:PHE:HB2    | 21:W:107:HIS:HA    | 2.03                     | 0.40              |
| 23:Y:135:VAL:O     | 23:Y:139:MET:HG3   | 2.21                     | 0.40              |
| 25:AA:1362:G:H2'   | 25:AA:1363:C:C6    | 2.57                     | 0.40              |
| 25:AA:1562:G:H1'   | 25:AA:1583:MA6:C2  | 2.46                     | 0.40              |
| 37:AM:29:ARG:HD2   | 37:AM:57:LEU:HD12  | 2.03                     | 0.40              |
| 43:AS:87:LEU:HB2   | 47:AW:117:GLY:HA3  | 2.03                     | 0.40              |
| 52:A1:98:ALA:O     | 52:A1:102:ASN:HB2  | 2.21                     | 0.40              |
| 52:A1:212:CYS:HB2  | 52:A1:218:ASN:CG   | 2.46                     | 0.40              |
| 52:A1:255:ASN:N    | 52:A1:259:GLU:OE1  | 2.54                     | 0.40              |
| 62:4:76:CYS:SG     | 62:4:98:HIS:CE1    | 3.14                     | 0.40              |
| 65:7:152:CYS:HB2   | 65:7:260:PHE:CD2   | 2.57                     | 0.40              |
| 70:c:69:HIS:NE2    | 70:c:73:GLN:OE1    | 2.54                     | 0.40              |
| 70:c:166:VAL:HG11  | 70:c:192:GLN:HG3   | 2.03                     | 0.40              |
| 71:d:189:LEU:HD21  | 71:d:219:ARG:NE    | 2.37                     | 0.40              |
| 73:f:121:VAL:HG22  | 73:f:159:ILE:HG22  | 2.04                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed      | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|------------|---------|----------|-------------|-----|
| 3   | D     | 236/305 (77%) | 227 (96%)  | 9 (4%)  | 0        | 100         | 100 |
| 4   | E     | 303/348 (87%) | 299 (99%)  | 4 (1%)  | 0        | 100         | 100 |
| 5   | F     | 250/311 (80%) | 247 (99%)  | 3 (1%)  | 0        | 100         | 100 |
| 6   | H     | 98/267 (37%)  | 97 (99%)   | 1 (1%)  | 0        | 100         | 100 |
| 7   | I     | 167/261 (64%) | 162 (97%)  | 5 (3%)  | 0        | 100         | 100 |
| 8   | J     | 173/192 (90%) | 172 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 9   | K     | 176/178 (99%) | 173 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 10  | L     | 113/145 (78%) | 111 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 11  | M     | 287/296 (97%) | 280 (98%)  | 7 (2%)  | 0        | 100         | 100 |
| 12  | N     | 220/251 (88%) | 218 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 13  | O     | 152/175 (87%) | 149 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 14  | P     | 142/180 (79%) | 136 (96%)  | 6 (4%)  | 0        | 100         | 100 |
| 15  | Q     | 237/292 (81%) | 232 (98%)  | 4 (2%)  | 1 (0%)   | 30          | 65  |
| 16  | R     | 138/149 (93%) | 136 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 17  | S     | 159/205 (78%) | 156 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 18  | T     | 164/206 (80%) | 160 (98%)  | 4 (2%)  | 0        | 100         | 100 |
| 19  | U     | 151/153 (99%) | 150 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 20  | V     | 203/216 (94%) | 196 (97%)  | 7 (3%)  | 0        | 100         | 100 |
| 21  | W     | 114/148 (77%) | 113 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 22  | X     | 242/256 (94%) | 236 (98%)  | 6 (2%)  | 0        | 100         | 100 |
| 23  | Y     | 179/250 (72%) | 179 (100%) | 0       | 0        | 100         | 100 |
| 24  | Z     | 120/161 (74%) | 119 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 26  | AB    | 223/296 (75%) | 217 (97%)  | 6 (3%)  | 0        | 100         | 100 |
| 27  | AC    | 130/167 (78%) | 129 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 28  | AD    | 341/430 (79%) | 335 (98%)  | 6 (2%)  | 0        | 100         | 100 |
| 29  | AE    | 120/125 (96%) | 119 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 30  | AF    | 206/242 (85%) | 204 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 31  | AG    | 307/396 (78%) | 300 (98%)  | 7 (2%)  | 0        | 100         | 100 |
| 32  | AH    | 138/201 (69%) | 135 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 33  | AI    | 134/194 (69%) | 130 (97%)  | 4 (3%)  | 0        | 100         | 100 |
| 34  | AJ    | 106/138 (77%) | 102 (96%)  | 4 (4%)  | 0        | 100         | 100 |
| 35  | AK    | 99/128 (77%)  | 97 (98%)   | 2 (2%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|------------|---------|----------|-------------|-----|
| 36  | AL    | 172/257 (67%) | 169 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 37  | AM    | 117/137 (85%) | 116 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 38  | AN    | 108/130 (83%) | 107 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 39  | AO    | 191/258 (74%) | 189 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 40  | AP    | 95/142 (67%)  | 95 (100%)  | 0       | 0        | 100         | 100 |
| 41  | AQ    | 85/87 (98%)   | 82 (96%)   | 3 (4%)  | 0        | 100         | 100 |
| 42  | AR    | 293/360 (81%) | 288 (98%)  | 5 (2%)  | 0        | 100         | 100 |
| 43  | AS    | 133/190 (70%) | 131 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 44  | AT    | 166/173 (96%) | 163 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 45  | AU    | 174/205 (85%) | 174 (100%) | 0       | 0        | 100         | 100 |
| 46  | AV    | 358/414 (86%) | 355 (99%)  | 3 (1%)  | 0        | 100         | 100 |
| 47  | AW    | 98/187 (52%)  | 98 (100%)  | 0       | 0        | 100         | 100 |
| 48  | AX    | 350/398 (88%) | 348 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 49  | AY    | 118/395 (30%) | 116 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 50  | AZ    | 98/106 (92%)  | 96 (98%)   | 2 (2%)  | 0        | 100         | 100 |
| 51  | A0    | 213/217 (98%) | 207 (97%)  | 6 (3%)  | 0        | 100         | 100 |
| 52  | A1    | 275/323 (85%) | 272 (99%)  | 3 (1%)  | 0        | 100         | 100 |
| 53  | A2    | 116/118 (98%) | 113 (97%)  | 3 (3%)  | 0        | 100         | 100 |
| 54  | A3    | 68/199 (34%)  | 67 (98%)   | 1 (2%)  | 0        | 100         | 100 |
| 55  | A4    | 527/689 (76%) | 520 (99%)  | 7 (1%)  | 0        | 100         | 100 |
| 58  | 0     | 108/188 (57%) | 107 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 59  | 1     | 51/65 (78%)   | 50 (98%)   | 1 (2%)  | 0        | 100         | 100 |
| 60  | 2     | 44/92 (48%)   | 44 (100%)  | 0       | 0        | 100         | 100 |
| 61  | 3     | 93/188 (50%)  | 93 (100%)  | 0       | 0        | 100         | 100 |
| 62  | 4     | 36/103 (35%)  | 36 (100%)  | 0       | 0        | 100         | 100 |
| 63  | 5     | 392/423 (93%) | 386 (98%)  | 6 (2%)  | 0        | 100         | 100 |
| 64  | 6     | 352/380 (93%) | 347 (99%)  | 5 (1%)  | 0        | 100         | 100 |
| 65  | 7     | 292/338 (86%) | 282 (97%)  | 10 (3%) | 0        | 100         | 100 |
| 66  | 8     | 138/206 (67%) | 136 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 67  | 9     | 122/137 (89%) | 121 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 68  | a     | 96/142 (68%)  | 94 (98%)   | 2 (2%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Favoured    | Allowed  | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 69  | b     | 149/215 (69%)     | 145 (97%)   | 4 (3%)   | 0        | 100         | 100 |
| 70  | c     | 282/332 (85%)     | 279 (99%)   | 3 (1%)   | 0        | 100         | 100 |
| 71  | d     | 235/306 (77%)     | 232 (99%)   | 3 (1%)   | 0        | 100         | 100 |
| 72  | e     | 236/279 (85%)     | 229 (97%)   | 7 (3%)   | 0        | 100         | 100 |
| 73  | f     | 153/212 (72%)     | 151 (99%)   | 2 (1%)   | 0        | 100         | 100 |
| 74  | g     | 132/166 (80%)     | 132 (100%)  | 0        | 0        | 100         | 100 |
| 75  | h     | 108/158 (68%)     | 105 (97%)   | 3 (3%)   | 0        | 100         | 100 |
| 76  | i     | 95/128 (74%)      | 94 (99%)    | 1 (1%)   | 0        | 100         | 100 |
| 77  | j     | 92/123 (75%)      | 90 (98%)    | 2 (2%)   | 0        | 100         | 100 |
| 78  | k     | 93/112 (83%)      | 93 (100%)   | 0        | 0        | 100         | 100 |
| 79  | l     | 80/138 (58%)      | 79 (99%)    | 1 (1%)   | 0        | 100         | 100 |
| 80  | m     | 90/128 (70%)      | 89 (99%)    | 1 (1%)   | 0        | 100         | 100 |
| 81  | o     | 92/102 (90%)      | 91 (99%)    | 1 (1%)   | 0        | 100         | 100 |
| 82  | p     | 137/206 (66%)     | 137 (100%)  | 0        | 0        | 100         | 100 |
| 83  | q     | 131/222 (59%)     | 131 (100%)  | 0        | 0        | 100         | 100 |
| 84  | r     | 160/196 (82%)     | 159 (99%)   | 1 (1%)   | 0        | 100         | 100 |
| 85  | s     | 379/439 (86%)     | 372 (98%)   | 7 (2%)   | 0        | 100         | 100 |
| 86  | t     | 9/198 (4%)        | 9 (100%)    | 0        | 0        | 100         | 100 |
| All | All   | 13960/18169 (77%) | 13735 (98%) | 224 (2%) | 1 (0%)   | 100         | 100 |

All (1) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 15  | Q     | 62  | ILE  |

### 5.3.2 Protein sidechains ⓘ

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

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



| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 3   | D     | 192/245 (78%)  | 191 (100%) | 1 (0%)   | 81          | 89  |
| 4   | E     | 260/290 (90%)  | 259 (100%) | 1 (0%)   | 84          | 90  |
| 5   | F     | 219/262 (84%)  | 218 (100%) | 1 (0%)   | 81          | 89  |
| 6   | H     | 90/228 (40%)   | 88 (98%)   | 2 (2%)   | 45          | 74  |
| 7   | I     | 155/232 (67%)  | 155 (100%) | 0        | 100         | 100 |
| 8   | J     | 138/150 (92%)  | 137 (99%)  | 1 (1%)   | 76          | 86  |
| 9   | K     | 155/155 (100%) | 155 (100%) | 0        | 100         | 100 |
| 10  | L     | 98/124 (79%)   | 98 (100%)  | 0        | 100         | 100 |
| 11  | M     | 245/249 (98%)  | 244 (100%) | 1 (0%)   | 84          | 90  |
| 12  | N     | 189/211 (90%)  | 188 (100%) | 1 (0%)   | 81          | 89  |
| 13  | O     | 134/150 (89%)  | 132 (98%)  | 2 (2%)   | 57          | 80  |
| 14  | P     | 126/155 (81%)  | 125 (99%)  | 1 (1%)   | 73          | 86  |
| 15  | Q     | 221/256 (86%)  | 220 (100%) | 1 (0%)   | 81          | 89  |
| 16  | R     | 118/126 (94%)  | 118 (100%) | 0        | 100         | 100 |
| 17  | S     | 146/180 (81%)  | 145 (99%)  | 1 (1%)   | 76          | 86  |
| 18  | T     | 146/176 (83%)  | 146 (100%) | 0        | 100         | 100 |
| 19  | U     | 134/134 (100%) | 134 (100%) | 0        | 100         | 100 |
| 20  | V     | 183/191 (96%)  | 183 (100%) | 0        | 100         | 100 |
| 21  | W     | 94/119 (79%)   | 93 (99%)   | 1 (1%)   | 65          | 83  |
| 22  | X     | 220/229 (96%)  | 220 (100%) | 0        | 100         | 100 |
| 23  | Y     | 163/223 (73%)  | 162 (99%)  | 1 (1%)   | 78          | 88  |
| 24  | Z     | 113/147 (77%)  | 112 (99%)  | 1 (1%)   | 70          | 85  |
| 26  | AB    | 198/249 (80%)  | 198 (100%) | 0        | 100         | 100 |
| 27  | AC    | 115/143 (80%)  | 114 (99%)  | 1 (1%)   | 70          | 85  |
| 28  | AD    | 286/357 (80%)  | 286 (100%) | 0        | 100         | 100 |
| 29  | AE    | 104/107 (97%)  | 104 (100%) | 0        | 100         | 100 |
| 30  | AF    | 185/209 (88%)  | 185 (100%) | 0        | 100         | 100 |
| 31  | AG    | 270/342 (79%)  | 270 (100%) | 0        | 100         | 100 |
| 32  | AH    | 130/180 (72%)  | 128 (98%)  | 2 (2%)   | 57          | 80  |
| 33  | AI    | 104/146 (71%)  | 104 (100%) | 0        | 100         | 100 |
| 34  | AJ    | 93/118 (79%)   | 92 (99%)   | 1 (1%)   | 65          | 83  |
| 35  | AK    | 91/113 (80%)   | 91 (100%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 36  | AL    | 158/226 (70%)  | 156 (99%)  | 2 (1%)   | 61          | 81  |
| 37  | AM    | 97/113 (86%)   | 97 (100%)  | 0        | 100         | 100 |
| 38  | AN    | 96/115 (84%)   | 95 (99%)   | 1 (1%)   | 68          | 84  |
| 39  | AO    | 174/230 (76%)  | 173 (99%)  | 1 (1%)   | 78          | 88  |
| 40  | AP    | 88/123 (72%)   | 88 (100%)  | 0        | 100         | 100 |
| 41  | AQ    | 78/78 (100%)   | 78 (100%)  | 0        | 100         | 100 |
| 42  | AR    | 264/318 (83%)  | 263 (100%) | 1 (0%)   | 84          | 90  |
| 43  | AS    | 116/164 (71%)  | 116 (100%) | 0        | 100         | 100 |
| 44  | AT    | 153/157 (98%)  | 152 (99%)  | 1 (1%)   | 76          | 86  |
| 45  | AU    | 152/174 (87%)  | 152 (100%) | 0        | 100         | 100 |
| 46  | AV    | 325/364 (89%)  | 325 (100%) | 0        | 100         | 100 |
| 47  | AW    | 87/158 (55%)   | 87 (100%)  | 0        | 100         | 100 |
| 48  | AX    | 311/351 (89%)  | 310 (100%) | 1 (0%)   | 86          | 91  |
| 49  | AY    | 111/357 (31%)  | 111 (100%) | 0        | 100         | 100 |
| 50  | AZ    | 90/95 (95%)    | 90 (100%)  | 0        | 100         | 100 |
| 51  | A0    | 188/189 (100%) | 188 (100%) | 0        | 100         | 100 |
| 52  | A1    | 255/291 (88%)  | 255 (100%) | 0        | 100         | 100 |
| 53  | A2    | 100/100 (100%) | 100 (100%) | 0        | 100         | 100 |
| 54  | A3    | 65/166 (39%)   | 65 (100%)  | 0        | 100         | 100 |
| 55  | A4    | 479/609 (79%)  | 475 (99%)  | 4 (1%)   | 73          | 86  |
| 58  | 0     | 99/164 (60%)   | 98 (99%)   | 1 (1%)   | 68          | 84  |
| 59  | 1     | 50/60 (83%)    | 50 (100%)  | 0        | 100         | 100 |
| 60  | 2     | 40/72 (56%)    | 39 (98%)   | 1 (2%)   | 42          | 72  |
| 61  | 3     | 88/166 (53%)   | 88 (100%)  | 0        | 100         | 100 |
| 62  | 4     | 37/89 (42%)    | 37 (100%)  | 0        | 100         | 100 |
| 63  | 5     | 353/368 (96%)  | 350 (99%)  | 3 (1%)   | 73          | 86  |
| 64  | 6     | 313/332 (94%)  | 313 (100%) | 0        | 100         | 100 |
| 65  | 7     | 270/303 (89%)  | 269 (100%) | 1 (0%)   | 84          | 90  |
| 66  | 8     | 129/190 (68%)  | 129 (100%) | 0        | 100         | 100 |
| 67  | 9     | 104/112 (93%)  | 104 (100%) | 0        | 100         | 100 |
| 68  | a     | 96/133 (72%)   | 96 (100%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Rotameric    | Outliers | Percentiles |     |
|-----|-------|-------------------|--------------|----------|-------------|-----|
| 69  | b     | 132/185 (71%)     | 132 (100%)   | 0        | 100         | 100 |
| 70  | c     | 251/288 (87%)     | 250 (100%)   | 1 (0%)   | 84          | 90  |
| 71  | d     | 223/274 (81%)     | 222 (100%)   | 1 (0%)   | 84          | 90  |
| 72  | e     | 207/236 (88%)     | 205 (99%)    | 2 (1%)   | 68          | 84  |
| 73  | f     | 139/188 (74%)     | 139 (100%)   | 0        | 100         | 100 |
| 74  | g     | 124/148 (84%)     | 124 (100%)   | 0        | 100         | 100 |
| 75  | h     | 104/148 (70%)     | 104 (100%)   | 0        | 100         | 100 |
| 76  | i     | 86/110 (78%)      | 86 (100%)    | 0        | 100         | 100 |
| 77  | j     | 74/97 (76%)       | 74 (100%)    | 0        | 100         | 100 |
| 78  | k     | 81/90 (90%)       | 81 (100%)    | 0        | 100         | 100 |
| 79  | l     | 76/116 (66%)      | 76 (100%)    | 0        | 100         | 100 |
| 80  | m     | 85/113 (75%)      | 85 (100%)    | 0        | 100         | 100 |
| 81  | o     | 80/87 (92%)       | 80 (100%)    | 0        | 100         | 100 |
| 82  | p     | 132/181 (73%)     | 132 (100%)   | 0        | 100         | 100 |
| 83  | q     | 114/178 (64%)     | 114 (100%)   | 0        | 100         | 100 |
| 84  | r     | 147/169 (87%)     | 147 (100%)   | 0        | 100         | 100 |
| 85  | s     | 338/381 (89%)     | 338 (100%)   | 0        | 100         | 100 |
| 86  | t     | 6/158 (4%)        | 6 (100%)     | 0        | 100         | 100 |
| All | All   | 12480/15710 (79%) | 12439 (100%) | 41 (0%)  | 84          | 91  |

All (41) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | D     | 226 | ILE  |
| 4   | E     | 285 | VAL  |
| 5   | F     | 94  | ASP  |
| 6   | H     | 83  | VAL  |
| 6   | H     | 102 | VAL  |
| 8   | J     | 104 | THR  |
| 11  | M     | 174 | VAL  |
| 12  | N     | 59  | VAL  |
| 13  | O     | 52  | MET  |
| 13  | O     | 93  | LEU  |
| 14  | P     | 103 | VAL  |
| 15  | Q     | 69  | VAL  |
| 17  | S     | 164 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 21  | W     | 131 | VAL  |
| 23  | Y     | 205 | VAL  |
| 24  | Z     | 99  | VAL  |
| 27  | AC    | 37  | ASN  |
| 32  | AH    | 148 | LEU  |
| 32  | AH    | 184 | ILE  |
| 34  | AJ    | 115 | THR  |
| 36  | AL    | 177 | VAL  |
| 36  | AL    | 213 | VAL  |
| 38  | AN    | 88  | VAL  |
| 39  | AO    | 167 | ILE  |
| 42  | AR    | 107 | THR  |
| 44  | AT    | 92  | THR  |
| 48  | AX    | 51  | THR  |
| 55  | A4    | 58  | VAL  |
| 55  | A4    | 309 | PHE  |
| 55  | A4    | 379 | PHE  |
| 55  | A4    | 508 | VAL  |
| 58  | 0     | 153 | THR  |
| 60  | 2     | 92  | HIS  |
| 63  | 5     | 180 | ILE  |
| 63  | 5     | 262 | ILE  |
| 63  | 5     | 307 | ASP  |
| 65  | 7     | 62  | THR  |
| 70  | c     | 307 | PHE  |
| 71  | d     | 81  | THR  |
| 72  | e     | 113 | ASP  |
| 72  | e     | 223 | THR  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (151) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | D     | 168 | HIS  |
| 3   | D     | 276 | HIS  |
| 4   | E     | 52  | HIS  |
| 4   | E     | 63  | GLN  |
| 4   | E     | 174 | GLN  |
| 4   | E     | 280 | HIS  |
| 5   | F     | 223 | HIS  |
| 6   | H     | 121 | ASN  |
| 7   | I     | 36  | HIS  |
| 7   | I     | 43  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | I     | 100 | GLN  |
| 7   | I     | 119 | HIS  |
| 7   | I     | 151 | ASN  |
| 8   | J     | 54  | ASN  |
| 9   | K     | 40  | GLN  |
| 9   | K     | 74  | GLN  |
| 10  | L     | 52  | HIS  |
| 10  | L     | 59  | HIS  |
| 11  | M     | 71  | GLN  |
| 11  | M     | 84  | ASN  |
| 12  | N     | 237 | HIS  |
| 13  | O     | 100 | GLN  |
| 15  | Q     | 139 | GLN  |
| 15  | Q     | 158 | GLN  |
| 15  | Q     | 172 | GLN  |
| 18  | T     | 73  | GLN  |
| 18  | T     | 204 | HIS  |
| 19  | U     | 74  | HIS  |
| 19  | U     | 98  | GLN  |
| 19  | U     | 136 | GLN  |
| 20  | V     | 18  | HIS  |
| 22  | X     | 240 | GLN  |
| 23  | Y     | 225 | ASN  |
| 24  | Z     | 100 | HIS  |
| 26  | AB    | 64  | ASN  |
| 26  | AB    | 134 | HIS  |
| 26  | AB    | 201 | ASN  |
| 26  | AB    | 228 | ASN  |
| 27  | AC    | 64  | HIS  |
| 27  | AC    | 130 | HIS  |
| 27  | AC    | 156 | GLN  |
| 28  | AD    | 155 | GLN  |
| 28  | AD    | 317 | HIS  |
| 28  | AD    | 415 | GLN  |
| 30  | AF    | 147 | GLN  |
| 31  | AG    | 77  | GLN  |
| 31  | AG    | 90  | ASN  |
| 31  | AG    | 135 | GLN  |
| 31  | AG    | 176 | GLN  |
| 31  | AG    | 261 | GLN  |
| 31  | AG    | 384 | GLN  |
| 32  | AH    | 125 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 33  | AI    | 98  | GLN  |
| 34  | AJ    | 100 | HIS  |
| 34  | AJ    | 105 | HIS  |
| 34  | AJ    | 116 | GLN  |
| 34  | AJ    | 134 | HIS  |
| 35  | AK    | 117 | HIS  |
| 39  | AO    | 111 | HIS  |
| 39  | AO    | 125 | GLN  |
| 39  | AO    | 130 | HIS  |
| 39  | AO    | 147 | HIS  |
| 39  | AO    | 169 | GLN  |
| 39  | AO    | 225 | GLN  |
| 41  | AQ    | 15  | GLN  |
| 42  | AR    | 110 | GLN  |
| 42  | AR    | 194 | GLN  |
| 42  | AR    | 214 | ASN  |
| 42  | AR    | 288 | GLN  |
| 43  | AS    | 66  | HIS  |
| 43  | AS    | 82  | GLN  |
| 44  | AT    | 14  | GLN  |
| 44  | AT    | 63  | GLN  |
| 46  | AV    | 78  | ASN  |
| 46  | AV    | 237 | GLN  |
| 46  | AV    | 238 | GLN  |
| 46  | AV    | 380 | GLN  |
| 48  | AX    | 81  | HIS  |
| 48  | AX    | 110 | HIS  |
| 48  | AX    | 235 | ASN  |
| 48  | AX    | 312 | GLN  |
| 50  | AZ    | 54  | ASN  |
| 50  | AZ    | 76  | GLN  |
| 51  | A0    | 133 | HIS  |
| 53  | A2    | 71  | GLN  |
| 55  | A4    | 90  | GLN  |
| 55  | A4    | 129 | GLN  |
| 55  | A4    | 136 | HIS  |
| 55  | A4    | 189 | ASN  |
| 55  | A4    | 257 | HIS  |
| 55  | A4    | 453 | HIS  |
| 55  | A4    | 545 | GLN  |
| 58  | 0     | 115 | HIS  |
| 58  | 0     | 120 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 58  | 0     | 188 | ASN  |
| 59  | 1     | 52  | GLN  |
| 63  | 5     | 150 | GLN  |
| 63  | 5     | 160 | HIS  |
| 63  | 5     | 275 | ASN  |
| 63  | 5     | 302 | HIS  |
| 63  | 5     | 384 | GLN  |
| 64  | 6     | 320 | GLN  |
| 65  | 7     | 247 | ASN  |
| 65  | 7     | 298 | GLN  |
| 66  | 8     | 158 | HIS  |
| 67  | 9     | 52  | GLN  |
| 68  | a     | 46  | ASN  |
| 68  | a     | 71  | HIS  |
| 68  | a     | 126 | HIS  |
| 70  | c     | 80  | GLN  |
| 70  | c     | 118 | ASN  |
| 70  | c     | 128 | GLN  |
| 70  | c     | 168 | HIS  |
| 70  | c     | 192 | GLN  |
| 70  | c     | 204 | GLN  |
| 70  | c     | 222 | GLN  |
| 71  | d     | 149 | HIS  |
| 71  | d     | 204 | ASN  |
| 72  | e     | 67  | GLN  |
| 72  | e     | 75  | GLN  |
| 72  | e     | 106 | HIS  |
| 72  | e     | 175 | GLN  |
| 72  | e     | 212 | HIS  |
| 72  | e     | 219 | GLN  |
| 72  | e     | 252 | HIS  |
| 72  | e     | 271 | GLN  |
| 73  | f     | 158 | GLN  |
| 74  | g     | 141 | ASN  |
| 76  | i     | 120 | HIS  |
| 78  | k     | 80  | HIS  |
| 79  | l     | 82  | GLN  |
| 79  | l     | 124 | GLN  |
| 79  | l     | 125 | ASN  |
| 79  | l     | 135 | ASN  |
| 80  | m     | 65  | HIS  |
| 80  | m     | 101 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 80  | m     | 108 | GLN  |
| 81  | o     | 21  | HIS  |
| 81  | o     | 58  | GLN  |
| 81  | o     | 85  | HIS  |
| 81  | o     | 94  | HIS  |
| 82  | p     | 123 | HIS  |
| 82  | p     | 190 | GLN  |
| 83  | q     | 81  | GLN  |
| 84  | r     | 79  | HIS  |
| 84  | r     | 96  | HIS  |
| 85  | s     | 152 | GLN  |
| 85  | s     | 179 | GLN  |
| 85  | s     | 240 | GLN  |
| 85  | s     | 358 | GLN  |
| 85  | s     | 397 | GLN  |

### 5.3.3 RNA [i](#)

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | A     | 1520/1561 (97%) | 258 (16%)         | 3 (0%)          |
| 2   | B     | 71/72 (98%)     | 16 (22%)          | 0               |
| 25  | AA    | 953/954 (99%)   | 148 (15%)         | 2 (0%)          |
| 56  | Ax    | 62/71 (87%)     | 11 (17%)          | 0               |
| 57  | Az    | 7/8 (87%)       | 1 (14%)           | 0               |
| All | All   | 2613/2666 (98%) | 434 (16%)         | 5 (0%)          |

All (434) RNA backbone outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1681 | G    |
| 1   | A     | 1689 | C    |
| 1   | A     | 1691 | C    |
| 1   | A     | 1693 | C    |
| 1   | A     | 1694 | U    |
| 1   | A     | 1699 | C    |
| 1   | A     | 1700 | U    |
| 1   | A     | 1704 | U    |
| 1   | A     | 1707 | C    |
| 1   | A     | 1708 | A    |
| 1   | A     | 1709 | G    |
| 1   | A     | 1711 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1715 | C    |
| 1   | A     | 1724 | A    |
| 1   | A     | 1727 | A    |
| 1   | A     | 1733 | C    |
| 1   | A     | 1735 | A    |
| 1   | A     | 1736 | A    |
| 1   | A     | 1748 | G    |
| 1   | A     | 1761 | A    |
| 1   | A     | 1763 | A    |
| 1   | A     | 1764 | C    |
| 1   | A     | 1765 | C    |
| 1   | A     | 1777 | A    |
| 1   | A     | 1805 | A    |
| 1   | A     | 1807 | U    |
| 1   | A     | 1808 | A    |
| 1   | A     | 1821 | A    |
| 1   | A     | 1827 | C    |
| 1   | A     | 1828 | A    |
| 1   | A     | 1829 | A    |
| 1   | A     | 1832 | A    |
| 1   | A     | 1836 | A    |
| 1   | A     | 1844 | A    |
| 1   | A     | 1854 | U    |
| 1   | A     | 1855 | A    |
| 1   | A     | 1856 | A    |
| 1   | A     | 1860 | A    |
| 1   | A     | 1868 | G    |
| 1   | A     | 1869 | A    |
| 1   | A     | 1878 | U    |
| 1   | A     | 1882 | A    |
| 1   | A     | 1885 | A    |
| 1   | A     | 1892 | A    |
| 1   | A     | 1893 | A    |
| 1   | A     | 1903 | C    |
| 1   | A     | 1909 | A    |
| 1   | A     | 1918 | G    |
| 1   | A     | 1935 | A    |
| 1   | A     | 1937 | A    |
| 1   | A     | 1938 | A    |
| 1   | A     | 1940 | A    |
| 1   | A     | 1958 | G    |
| 1   | A     | 1975 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1985 | G    |
| 1   | A     | 1987 | G    |
| 1   | A     | 1992 | C    |
| 1   | A     | 1994 | A    |
| 1   | A     | 2003 | A    |
| 1   | A     | 2015 | G    |
| 1   | A     | 2022 | G    |
| 1   | A     | 2030 | U    |
| 1   | A     | 2031 | A    |
| 1   | A     | 2036 | C    |
| 1   | A     | 2037 | U    |
| 1   | A     | 2039 | A    |
| 1   | A     | 2054 | U    |
| 1   | A     | 2060 | A    |
| 1   | A     | 2070 | C    |
| 1   | A     | 2071 | U    |
| 1   | A     | 2074 | A    |
| 1   | A     | 2079 | C    |
| 1   | A     | 2092 | C    |
| 1   | A     | 2098 | G    |
| 1   | A     | 2099 | U    |
| 1   | A     | 2111 | C    |
| 1   | A     | 2113 | G    |
| 1   | A     | 2125 | C    |
| 1   | A     | 2126 | U    |
| 1   | A     | 2131 | A    |
| 1   | A     | 2147 | G    |
| 1   | A     | 2159 | U    |
| 1   | A     | 2160 | A    |
| 1   | A     | 2161 | A    |
| 1   | A     | 2162 | C    |
| 1   | A     | 2163 | A    |
| 1   | A     | 2166 | C    |
| 1   | A     | 2174 | G    |
| 1   | A     | 2175 | C    |
| 1   | A     | 2181 | A    |
| 1   | A     | 2182 | G    |
| 1   | A     | 2196 | A    |
| 1   | A     | 2198 | A    |
| 1   | A     | 2199 | A    |
| 1   | A     | 2211 | U    |
| 1   | A     | 2214 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 2219 | C    |
| 1   | A     | 2220 | A    |
| 1   | A     | 2221 | C    |
| 1   | A     | 2223 | A    |
| 1   | A     | 2224 | C    |
| 1   | A     | 2225 | C    |
| 1   | A     | 2226 | U    |
| 1   | A     | 2227 | A    |
| 1   | A     | 2230 | A    |
| 1   | A     | 2237 | A    |
| 1   | A     | 2241 | A    |
| 1   | A     | 2243 | A    |
| 1   | A     | 2245 | A    |
| 1   | A     | 2246 | A    |
| 1   | A     | 2260 | A    |
| 1   | A     | 2262 | C    |
| 1   | A     | 2263 | C    |
| 1   | A     | 2284 | C    |
| 1   | A     | 2297 | A    |
| 1   | A     | 2299 | U    |
| 1   | A     | 2300 | G    |
| 1   | A     | 2302 | U    |
| 1   | A     | 2317 | G    |
| 1   | A     | 2321 | A    |
| 1   | A     | 2322 | C    |
| 1   | A     | 2331 | C    |
| 1   | A     | 2332 | C    |
| 1   | A     | 2345 | G    |
| 1   | A     | 2349 | G    |
| 1   | A     | 2350 | A    |
| 1   | A     | 2354 | A    |
| 1   | A     | 2357 | C    |
| 1   | A     | 2363 | A    |
| 1   | A     | 2372 | U    |
| 1   | A     | 2374 | A    |
| 1   | A     | 2381 | A    |
| 1   | A     | 2388 | A    |
| 1   | A     | 2390 | A    |
| 1   | A     | 2391 | A    |
| 1   | A     | 2393 | C    |
| 1   | A     | 2396 | C    |
| 1   | A     | 2397 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 2404 | U    |
| 1   | A     | 2406 | A    |
| 1   | A     | 2407 | U    |
| 1   | A     | 2414 | C    |
| 1   | A     | 2415 | C    |
| 1   | A     | 2446 | A    |
| 1   | A     | 2451 | A    |
| 1   | A     | 2458 | A    |
| 1   | A     | 2478 | G    |
| 1   | A     | 2480 | A    |
| 1   | A     | 2485 | U    |
| 1   | A     | 2493 | C    |
| 1   | A     | 2504 | A    |
| 1   | A     | 2520 | C    |
| 1   | A     | 2521 | A    |
| 1   | A     | 2524 | A    |
| 1   | A     | 2527 | A    |
| 1   | A     | 2536 | G    |
| 1   | A     | 2540 | C    |
| 1   | A     | 2557 | C    |
| 1   | A     | 2558 | A    |
| 1   | A     | 2570 | C    |
| 1   | A     | 2592 | G    |
| 1   | A     | 2593 | G    |
| 1   | A     | 2594 | U    |
| 1   | A     | 2601 | A    |
| 1   | A     | 2603 | C    |
| 1   | A     | 2618 | U    |
| 1   | A     | 2627 | G    |
| 1   | A     | 2629 | A    |
| 1   | A     | 2630 | U    |
| 1   | A     | 2633 | A    |
| 1   | A     | 2635 | G    |
| 1   | A     | 2654 | U    |
| 1   | A     | 2683 | C    |
| 1   | A     | 2684 | C    |
| 1   | A     | 2686 | G    |
| 1   | A     | 2694 | A    |
| 1   | A     | 2695 | G    |
| 1   | A     | 2696 | A    |
| 1   | A     | 2706 | A    |
| 1   | A     | 2709 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 2715 | A    |
| 1   | A     | 2718 | C    |
| 1   | A     | 2719 | G    |
| 1   | A     | 2721 | G    |
| 1   | A     | 2722 | A    |
| 1   | A     | 2723 | A    |
| 1   | A     | 2724 | G    |
| 1   | A     | 2725 | A    |
| 1   | A     | 2732 | G    |
| 1   | A     | 2745 | A    |
| 1   | A     | 2810 | G    |
| 1   | A     | 2832 | A    |
| 1   | A     | 2833 | A    |
| 1   | A     | 2847 | C    |
| 1   | A     | 2864 | U    |
| 1   | A     | 2865 | C    |
| 1   | A     | 2882 | U    |
| 1   | A     | 2884 | C    |
| 1   | A     | 2885 | U    |
| 1   | A     | 2886 | A    |
| 1   | A     | 2887 | U    |
| 1   | A     | 2889 | C    |
| 1   | A     | 2893 | A    |
| 1   | A     | 2913 | A    |
| 1   | A     | 2917 | G    |
| 1   | A     | 2922 | A    |
| 1   | A     | 2928 | C    |
| 1   | A     | 2934 | G    |
| 1   | A     | 2935 | A    |
| 1   | A     | 2956 | A    |
| 1   | A     | 2965 | A    |
| 1   | A     | 2985 | C    |
| 1   | A     | 2989 | G    |
| 1   | A     | 2990 | A    |
| 1   | A     | 2992 | G    |
| 1   | A     | 2994 | U    |
| 1   | A     | 3005 | A    |
| 1   | A     | 3007 | C    |
| 1   | A     | 3016 | G    |
| 1   | A     | 3022 | G    |
| 1   | A     | 3041 | U    |
| 1   | A     | 3051 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 3053 | A    |
| 1   | A     | 3054 | G    |
| 1   | A     | 3060 | C    |
| 1   | A     | 3064 | A    |
| 1   | A     | 3069 | A    |
| 1   | A     | 3090 | G    |
| 1   | A     | 3096 | U    |
| 1   | A     | 3100 | U    |
| 1   | A     | 3102 | U    |
| 1   | A     | 3108 | U    |
| 1   | A     | 3109 | U    |
| 1   | A     | 3110 | C    |
| 1   | A     | 3112 | A    |
| 1   | A     | 3113 | A    |
| 1   | A     | 3122 | U    |
| 1   | A     | 3157 | C    |
| 1   | A     | 3158 | A    |
| 1   | A     | 3162 | C    |
| 1   | A     | 3168 | C    |
| 1   | A     | 3169 | C    |
| 1   | A     | 3172 | C    |
| 1   | A     | 3176 | A    |
| 1   | A     | 3180 | A    |
| 1   | A     | 3183 | U    |
| 1   | A     | 3190 | A    |
| 1   | A     | 3199 | U    |
| 1   | A     | 3200 | U    |
| 1   | A     | 3207 | A    |
| 1   | A     | 3209 | A    |
| 1   | A     | 3210 | C    |
| 1   | A     | 3212 | C    |
| 1   | A     | 3217 | A    |
| 1   | A     | 3218 | A    |
| 1   | A     | 3228 | U    |
| 1   | A     | 3229 | U    |
| 1   | A     | 3231 | U    |
| 2   | B     | 7    | G    |
| 2   | B     | 8    | U    |
| 2   | B     | 10   | 2MG  |
| 2   | B     | 16   | C    |
| 2   | B     | 21   | A    |
| 2   | B     | 45   | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | B     | 46  | A    |
| 2   | B     | 48  | U    |
| 2   | B     | 49  | U    |
| 2   | B     | 54  | C    |
| 2   | B     | 55  | U    |
| 2   | B     | 56  | U    |
| 2   | B     | 58  | A    |
| 2   | B     | 59  | A    |
| 2   | B     | 72  | G    |
| 2   | B     | 76  | A    |
| 25  | AA    | 651 | A    |
| 25  | AA    | 673 | U    |
| 25  | AA    | 680 | U    |
| 25  | AA    | 688 | A    |
| 25  | AA    | 695 | A    |
| 25  | AA    | 704 | U    |
| 25  | AA    | 721 | U    |
| 25  | AA    | 730 | A    |
| 25  | AA    | 737 | C    |
| 25  | AA    | 738 | A    |
| 25  | AA    | 753 | A    |
| 25  | AA    | 761 | A    |
| 25  | AA    | 766 | G    |
| 25  | AA    | 783 | A    |
| 25  | AA    | 791 | G    |
| 25  | AA    | 794 | U    |
| 25  | AA    | 796 | G    |
| 25  | AA    | 815 | C    |
| 25  | AA    | 830 | U    |
| 25  | AA    | 832 | U    |
| 25  | AA    | 835 | C    |
| 25  | AA    | 851 | A    |
| 25  | AA    | 860 | A    |
| 25  | AA    | 861 | U    |
| 25  | AA    | 866 | A    |
| 25  | AA    | 868 | C    |
| 25  | AA    | 869 | C    |
| 25  | AA    | 870 | C    |
| 25  | AA    | 871 | A    |
| 25  | AA    | 881 | A    |
| 25  | AA    | 883 | U    |
| 25  | AA    | 890 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 25  | AA    | 893  | G    |
| 25  | AA    | 903  | U    |
| 25  | AA    | 904  | C    |
| 25  | AA    | 907  | A    |
| 25  | AA    | 919  | A    |
| 25  | AA    | 923  | A    |
| 25  | AA    | 929  | A    |
| 25  | AA    | 930  | G    |
| 25  | AA    | 932  | C    |
| 25  | AA    | 939  | A    |
| 25  | AA    | 941  | G    |
| 25  | AA    | 942  | A    |
| 25  | AA    | 946  | U    |
| 25  | AA    | 947  | U    |
| 25  | AA    | 954  | C    |
| 25  | AA    | 960  | C    |
| 25  | AA    | 962  | C    |
| 25  | AA    | 967  | A    |
| 25  | AA    | 975  | A    |
| 25  | AA    | 993  | A    |
| 25  | AA    | 1002 | C    |
| 25  | AA    | 1010 | A    |
| 25  | AA    | 1015 | A    |
| 25  | AA    | 1031 | G    |
| 25  | AA    | 1042 | U    |
| 25  | AA    | 1047 | A    |
| 25  | AA    | 1049 | A    |
| 25  | AA    | 1065 | C    |
| 25  | AA    | 1081 | U    |
| 25  | AA    | 1082 | A    |
| 25  | AA    | 1094 | U    |
| 25  | AA    | 1098 | C    |
| 25  | AA    | 1103 | A    |
| 25  | AA    | 1105 | C    |
| 25  | AA    | 1106 | C    |
| 25  | AA    | 1107 | U    |
| 25  | AA    | 1109 | A    |
| 25  | AA    | 1118 | A    |
| 25  | AA    | 1119 | U    |
| 25  | AA    | 1120 | C    |
| 25  | AA    | 1121 | A    |
| 25  | AA    | 1137 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 25  | AA    | 1138 | G    |
| 25  | AA    | 1144 | U    |
| 25  | AA    | 1151 | C    |
| 25  | AA    | 1153 | C    |
| 25  | AA    | 1160 | A    |
| 25  | AA    | 1167 | A    |
| 25  | AA    | 1179 | G    |
| 25  | AA    | 1187 | U    |
| 25  | AA    | 1188 | A    |
| 25  | AA    | 1189 | U    |
| 25  | AA    | 1190 | C    |
| 25  | AA    | 1193 | U    |
| 25  | AA    | 1209 | C    |
| 25  | AA    | 1220 | A    |
| 25  | AA    | 1223 | C    |
| 25  | AA    | 1225 | C    |
| 25  | AA    | 1229 | U    |
| 25  | AA    | 1236 | C    |
| 25  | AA    | 1246 | U    |
| 25  | AA    | 1247 | G    |
| 25  | AA    | 1248 | C    |
| 25  | AA    | 1250 | C    |
| 25  | AA    | 1251 | A    |
| 25  | AA    | 1256 | A    |
| 25  | AA    | 1258 | A    |
| 25  | AA    | 1265 | C    |
| 25  | AA    | 1271 | C    |
| 25  | AA    | 1273 | G    |
| 25  | AA    | 1275 | A    |
| 25  | AA    | 1284 | U    |
| 25  | AA    | 1290 | C    |
| 25  | AA    | 1291 | U    |
| 25  | AA    | 1300 | A    |
| 25  | AA    | 1326 | A    |
| 25  | AA    | 1327 | G    |
| 25  | AA    | 1330 | C    |
| 25  | AA    | 1343 | A    |
| 25  | AA    | 1353 | A    |
| 25  | AA    | 1354 | A    |
| 25  | AA    | 1356 | A    |
| 25  | AA    | 1378 | C    |
| 25  | AA    | 1379 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 25  | AA    | 1387 | A    |
| 25  | AA    | 1390 | A    |
| 25  | AA    | 1391 | U    |
| 25  | AA    | 1405 | C    |
| 25  | AA    | 1407 | U    |
| 25  | AA    | 1430 | A    |
| 25  | AA    | 1481 | C    |
| 25  | AA    | 1482 | A    |
| 25  | AA    | 1494 | C    |
| 25  | AA    | 1507 | A    |
| 25  | AA    | 1512 | A    |
| 25  | AA    | 1519 | A    |
| 25  | AA    | 1522 | U    |
| 25  | AA    | 1525 | C    |
| 25  | AA    | 1526 | U    |
| 25  | AA    | 1527 | A    |
| 25  | AA    | 1533 | C    |
| 25  | AA    | 1536 | A    |
| 25  | AA    | 1537 | C    |
| 25  | AA    | 1539 | C    |
| 25  | AA    | 1540 | A    |
| 25  | AA    | 1541 | U    |
| 25  | AA    | 1551 | G    |
| 25  | AA    | 1557 | A    |
| 25  | AA    | 1564 | A    |
| 25  | AA    | 1568 | U    |
| 25  | AA    | 1571 | U    |
| 25  | AA    | 1582 | G    |
| 25  | AA    | 1584 | MA6  |
| 25  | AA    | 1594 | G    |
| 25  | AA    | 1595 | G    |
| 25  | AA    | 1599 | A    |
| 56  | Ax    | 2    | G    |
| 56  | Ax    | 3    | U    |
| 56  | Ax    | 34   | RSQ  |
| 56  | Ax    | 42   | G    |
| 56  | Ax    | 43   | A    |
| 56  | Ax    | 44   | A    |
| 56  | Ax    | 45   | A    |
| 56  | Ax    | 46   | A    |
| 56  | Ax    | 48   | U    |
| 56  | Ax    | 53   | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 56  | Ax    | 76  | A    |
| 57  | Az    | 11  | U    |

All (5) RNA pucker outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1692 | A    |
| 1   | A     | 2245 | A    |
| 1   | A     | 2349 | G    |
| 25  | AA    | 1255 | U    |
| 25  | AA    | 1539 | C    |

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

15 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 | $\# Z  > 2$ |
| 1   | PSU  | A     | 3067 | 1       | 18,21,22     | 0.47 | 0           | 21,30,33    | 0.62 | 1 (4%)      |
| 1   | OMU  | A     | 3039 | 88,1    | 19,22,23     | 0.21 | 0           | 25,31,34    | 0.41 | 0           |
| 1   | OMG  | A     | 3040 | 1       | 23,26,27     | 0.23 | 0           | 32,38,41    | 0.36 | 0           |
| 2   | 1MA  | B     | 9    | 2       | 21,25,26     | 0.76 | 1 (4%)      | 30,37,40    | 0.62 | 1 (3%)      |
| 25  | B8T  | AA    | 1486 | 25,87   | 19,22,23     | 0.25 | 0           | 25,31,34    | 0.29 | 0           |
| 2   | 2MG  | B     | 10   | 2       | 23,26,27     | 0.23 | 0           | 33,38,41    | 0.35 | 0           |
| 1   | OMG  | A     | 2815 | 88,1,56 | 23,26,27     | 0.23 | 0           | 32,38,41    | 0.37 | 0           |
| 2   | PSU  | B     | 39   | 2       | 18,21,22     | 0.45 | 0           | 21,30,33    | 0.56 | 0           |
| 25  | 5MC  | AA    | 1488 | 25      | 19,22,23     | 0.34 | 0           | 26,32,35    | 0.44 | 0           |
| 25  | MA6  | AA    | 1583 | 25      | 23,26,27     | 0.25 | 0           | 33,38,41    | 0.55 | 1 (3%)      |
| 33  | 5F0  | AI    | 184  | 33      | 8,8,9        | 0.51 | 0           | 8,9,11      | 0.97 | 1 (12%)     |
| 25  | MA6  | AA    | 1584 | 25      | 23,26,27     | 0.27 | 0           | 33,38,41    | 0.56 | 1 (3%)      |
| 56  | RSQ  | Ax    | 34   | 57,56   | 19,23,24     | 0.26 | 0           | 25,33,36    | 0.32 | 0           |
| 1   | 1MA  | A     | 2617 | 1       | 21,25,26     | 0.76 | 1 (4%)      | 30,37,40    | 0.63 | 1 (3%)      |
| 25  | 5MU  | AA    | 1076 | 25      | 19,22,23     | 0.23 | 0           | 27,32,35    | 0.29 | 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   |
|-----|------|-------|------|---------|---------|------------|---------|
| 1   | PSU  | A     | 3067 | 1       | -       | 0/7/25/26  | 0/2/2/2 |
| 1   | OMU  | A     | 3039 | 88,1    | -       | 0/9/27/28  | 0/2/2/2 |
| 1   | OMG  | A     | 3040 | 1       | -       | 0/9/27/28  | 0/3/3/3 |
| 2   | 1MA  | B     | 9    | 2       | -       | 0/7/25/26  | 0/3/3/3 |
| 25  | B8T  | AA    | 1486 | 25,87   | -       | 0/7/27/28  | 0/2/2/2 |
| 2   | 2MG  | B     | 10   | 2       | -       | 0/9/27/28  | 0/3/3/3 |
| 1   | OMG  | A     | 2815 | 88,1,56 | -       | 0/9/27/28  | 0/3/3/3 |
| 2   | PSU  | B     | 39   | 2       | -       | 0/7/25/26  | 0/2/2/2 |
| 25  | 5MC  | AA    | 1488 | 25      | -       | 0/7/25/26  | 0/2/2/2 |
| 25  | MA6  | AA    | 1583 | 25      | -       | 3/11/29/30 | 0/3/3/3 |
| 33  | 5F0  | AI    | 184  | 33      | -       | 6/9/9/10   | -       |
| 25  | MA6  | AA    | 1584 | 25      | -       | 4/11/29/30 | 0/3/3/3 |
| 56  | RSQ  | Ax    | 34   | 57,56   | -       | 1/9/27/28  | 0/2/2/2 |
| 1   | 1MA  | A     | 2617 | 1       | -       | 0/7/25/26  | 0/3/3/3 |
| 25  | 5MU  | AA    | 1076 | 25      | -       | 0/7/25/26  | 0/2/2/2 |

All (2) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 2   | B     | 9    | 1MA  | C6-N6 | 3.19 | 1.35        | 1.28     |
| 1   | A     | 2617 | 1MA  | C6-N6 | 3.15 | 1.35        | 1.28     |

All (6) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 33  | AI    | 184  | 5F0  | O-C-CB      | -2.28 | 118.75      | 125.38   |
| 25  | AA    | 1583 | MA6  | C2-N1-C6    | 2.24  | 117.30      | 111.83   |
| 25  | AA    | 1584 | MA6  | C2-N1-C6    | 2.22  | 117.25      | 111.83   |
| 1   | A     | 3067 | PSU  | O4'-C1'-C2' | 2.16  | 108.14      | 105.15   |
| 2   | B     | 9    | 1MA  | N1-C6-N6    | 2.13  | 125.07      | 119.71   |
| 1   | A     | 2617 | 1MA  | N1-C6-N6    | 2.12  | 125.04      | 119.71   |

There are no chirality outliers.

All (14) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       |
|-----|-------|------|------|-------------|
| 25  | AA    | 1583 | MA6  | C5-C6-N6-C9 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 25  | AA    | 1584 | MA6  | C5-C6-N6-C9     |
| 33  | AI    | 184  | 5F0  | O1-C1-CA-CB     |
| 33  | AI    | 184  | 5F0  | OD1-C1-CA-CB    |
| 33  | AI    | 184  | 5F0  | N-CA-CB-C       |
| 33  | AI    | 184  | 5F0  | C1-CA-CB-C      |
| 33  | AI    | 184  | 5F0  | O-C-CB-CA       |
| 25  | AA    | 1584 | MA6  | N1-C6-N6-C9     |
| 25  | AA    | 1583 | MA6  | N1-C6-N6-C9     |
| 33  | AI    | 184  | 5F0  | O1-C1-CA-N      |
| 25  | AA    | 1584 | MA6  | C5-C6-N6-C10    |
| 56  | Ax    | 34   | RSQ  | O4'-C4'-C5'-O5' |
| 25  | AA    | 1584 | MA6  | C4'-C5'-O5'-P   |
| 25  | AA    | 1583 | MA6  | C5-C6-N6-C10    |

There are no ring outliers.

5 monomers are involved in 8 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 25  | AA    | 1486 | B8T  | 1       | 0            |
| 1   | A     | 2815 | OMG  | 2       | 0            |
| 25  | AA    | 1488 | 5MC  | 2       | 0            |
| 25  | AA    | 1583 | MA6  | 3       | 0            |
| 25  | AA    | 1584 | MA6  | 1       | 0            |

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 273 ligands modelled in this entry, 264 are monoatomic - leaving 9 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 |
| 96  | GDP  | AX    | 503  | -     | 29,30,30     | 0.42 | 0        | 45,47,47    | 0.43 | 0        |
| 94  | FES  | AT    | 201  | 44,37 | 0,4,4        | -    | -        | -           |      |          |
| 95  | ATP  | AX    | 501  | 87    | 32,33,33     | 0.53 | 0        | 48,52,52    | 0.52 | 0        |
| 92  | SPD  | AA    | 1703 | -     | 9,9,9        | 0.28 | 0        | 8,8,8       | 0.85 | 0        |
| 90  | VAL  | B     | 101  | 2     | 4,6,7        | 0.53 | 0        | 6,7,9       | 0.93 | 0        |
| 94  | FES  | AP    | 201  | 29,40 | 0,4,4        | -    | -        | -           |      |          |
| 94  | FES  | r     | 201  | 7,84  | 0,4,4        | -    | -        | -           |      |          |
| 89  | G34  | A     | 6456 | -     | 40,40,40     | 0.50 | 0        | 61,64,64    | 1.08 | 3 (4%)   |
| 91  | NAD  | AA    | 1701 | 87    | 46,48,48     | 0.41 | 0        | 64,73,73    | 0.36 | 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   |
|-----|------|-------|------|-------|---------|------------|---------|
| 96  | GDP  | AX    | 503  | -     | -       | 0/16/32/32 | 0/3/3/3 |
| 94  | FES  | AT    | 201  | 44,37 | -       | -          | 0/1/1/1 |
| 95  | ATP  | AX    | 501  | 87    | -       | 0/22/38/38 | 0/3/3/3 |
| 92  | SPD  | AA    | 1703 | -     | -       | 0/7/7/7    | -       |
| 90  | VAL  | B     | 101  | 2     | -       | 0/5/6/8    | -       |
| 94  | FES  | AP    | 201  | 29,40 | -       | -          | 0/1/1/1 |
| 94  | FES  | r     | 201  | 7,84  | -       | -          | 0/1/1/1 |
| 89  | G34  | A     | 6456 | -     | -       | 2/12/94/94 | 0/6/5/5 |
| 91  | NAD  | AA    | 1701 | 87    | -       | 4/30/62/62 | 0/5/5/5 |

There are no bond length outliers.

All (3) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 89  | A     | 6456 | G34  | O1-C3-C2   | -3.30 | 120.80      | 125.52   |
| 89  | A     | 6456 | G34  | C15-C5-C14 | -2.97 | 105.77      | 108.81   |
| 89  | A     | 6456 | G34  | C1-C9-C10  | -2.68 | 107.44      | 110.55   |

There are no chirality outliers.

All (6) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 89  | A     | 6456 | G34  | C24-C23-S1-C22  |
| 91  | AA    | 1701 | NAD  | O4B-C4B-C5B-O5B |

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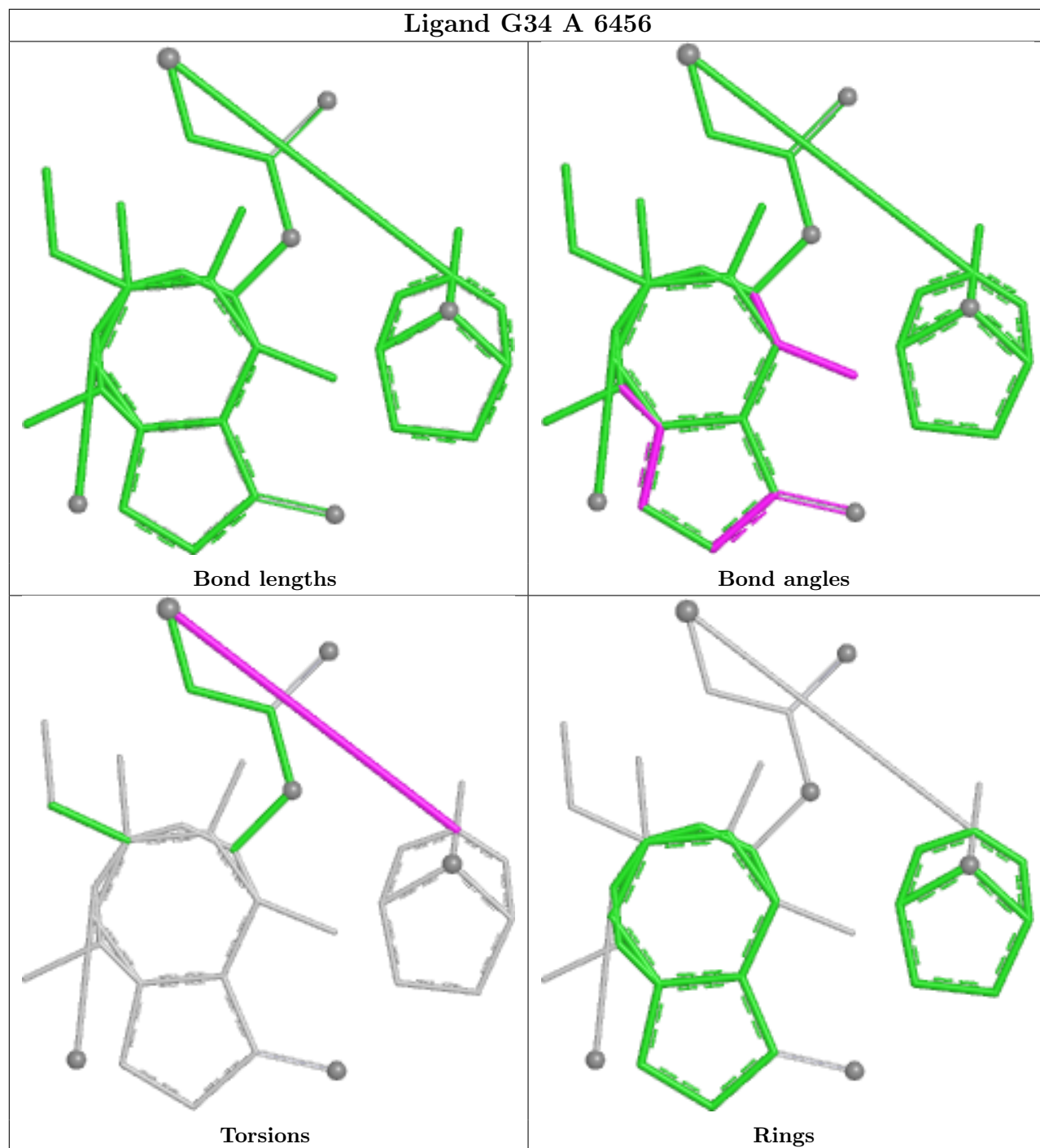
| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 91  | AA    | 1701 | NAD  | C3B-C4B-C5B-O5B |
| 89  | A     | 6456 | G34  | C29-C23-S1-C22  |
| 91  | AA    | 1701 | NAD  | C5D-O5D-PN-O1N  |
| 91  | AA    | 1701 | NAD  | PA-O3-PN-O2N    |

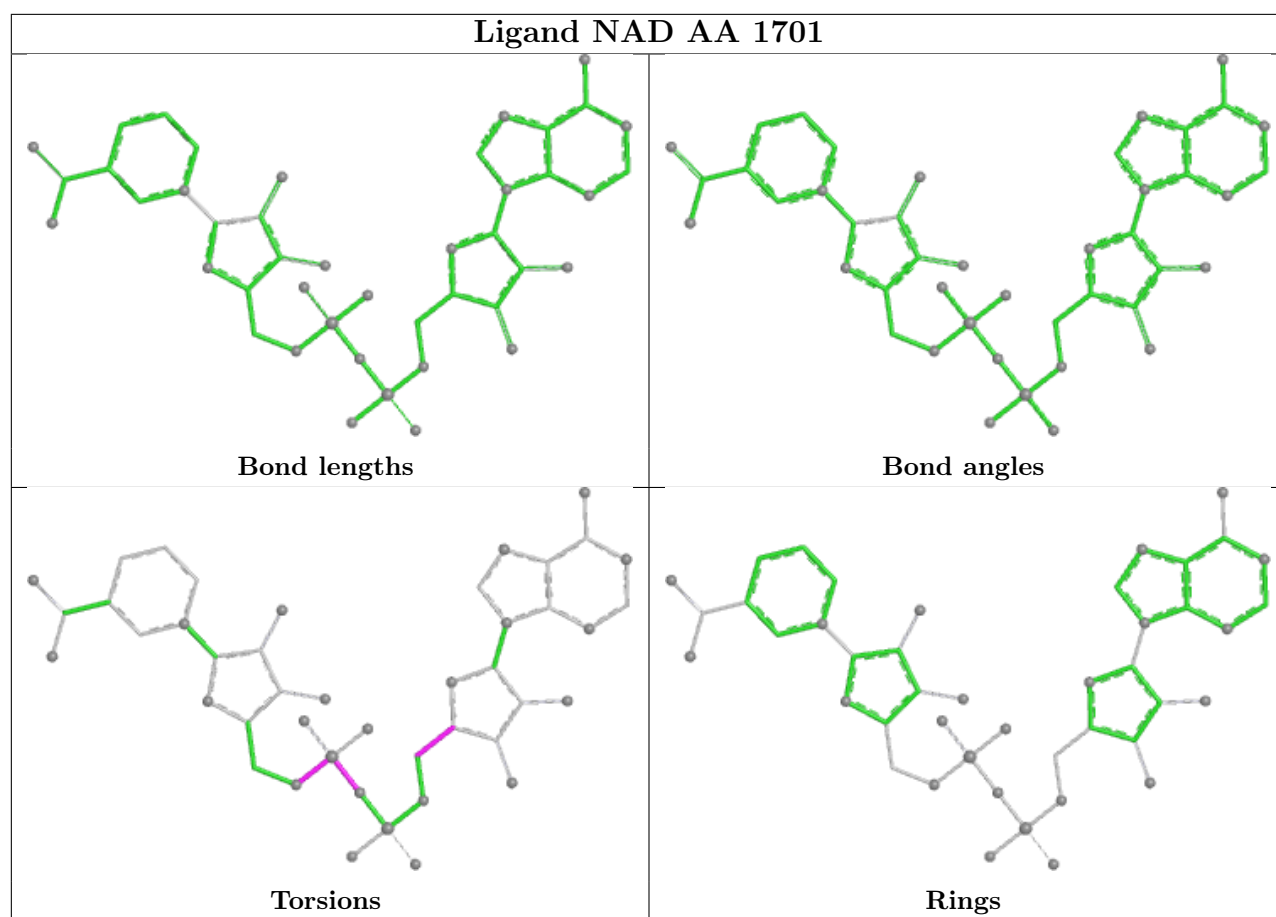
There are no ring outliers.

5 monomers are involved in 8 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 96  | AX    | 503  | GDP  | 1       | 0            |
| 95  | AX    | 501  | ATP  | 1       | 0            |
| 90  | B     | 101  | VAL  | 2       | 0            |
| 89  | A     | 6456 | G34  | 3       | 0            |
| 91  | AA    | 1701 | NAD  | 1       | 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.





## 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.



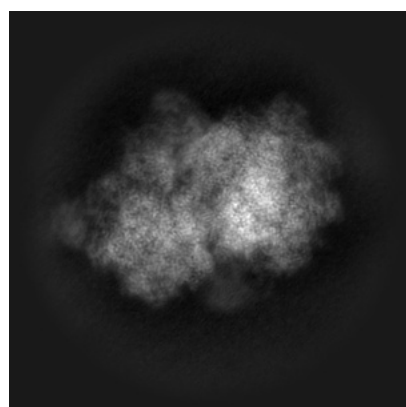
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-64554. These allow visual inspection of the internal detail of the map and identification of artifacts.

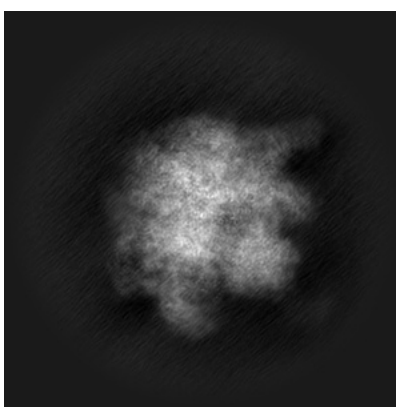
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

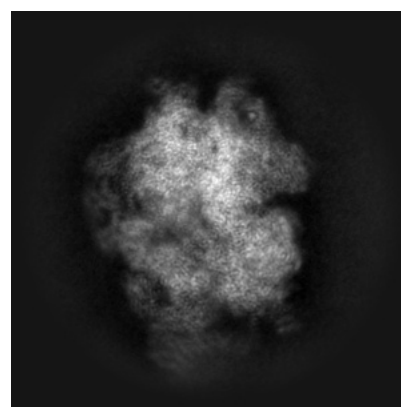
#### 6.1.1 Primary map



X



Y

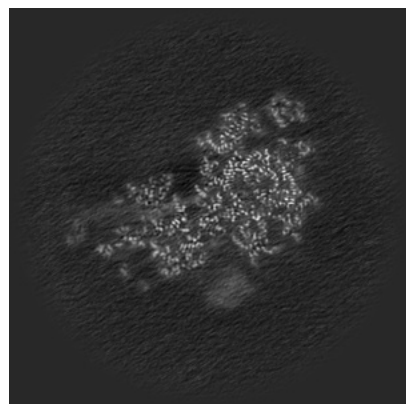


Z

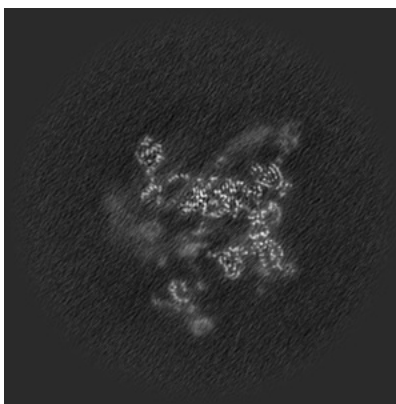
The images above show the map projected in three orthogonal directions.

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

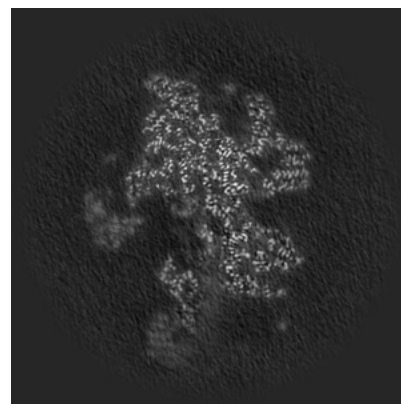
#### 6.2.1 Primary map



X Index: 256



Y Index: 256

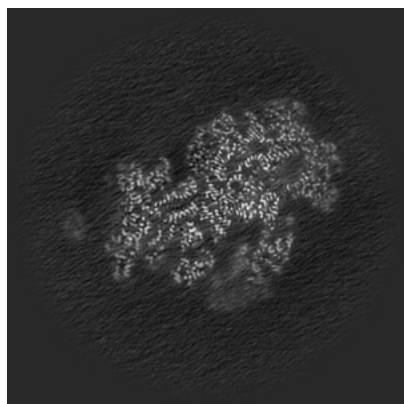


Z Index: 256

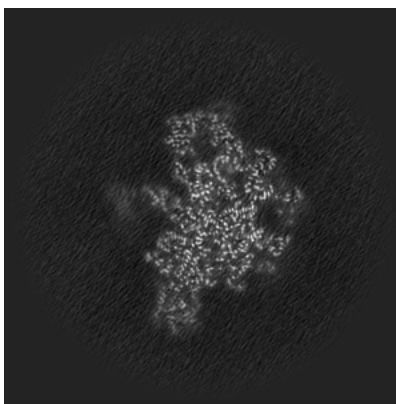
The images above show central slices of the map in three orthogonal directions.

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

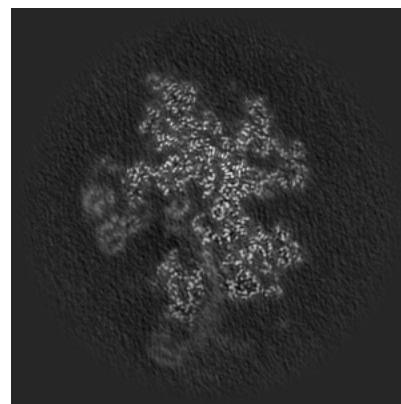
### 6.3.1 Primary map



X Index: 277



Y Index: 306

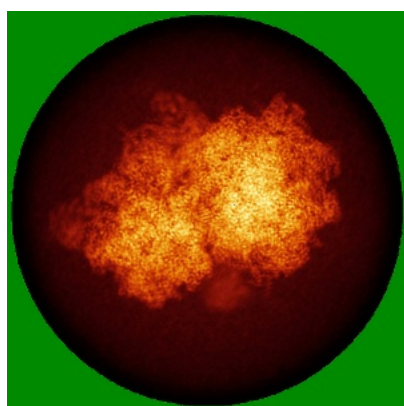


Z Index: 248

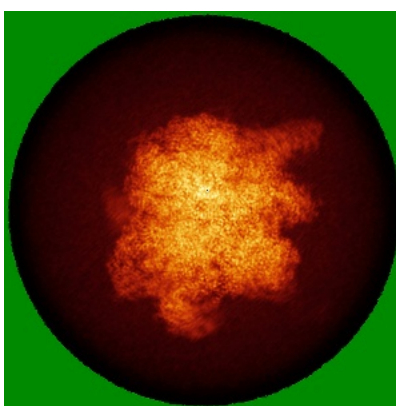
The images above show the largest variance slices of the map in three orthogonal directions.

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

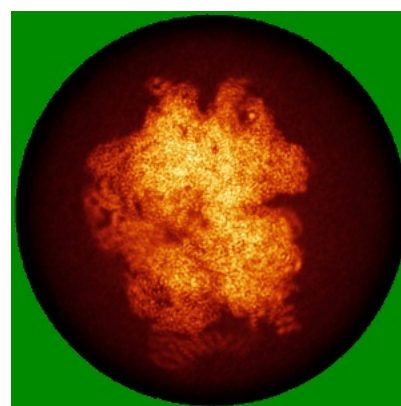
### 6.4.1 Primary map



X



Y

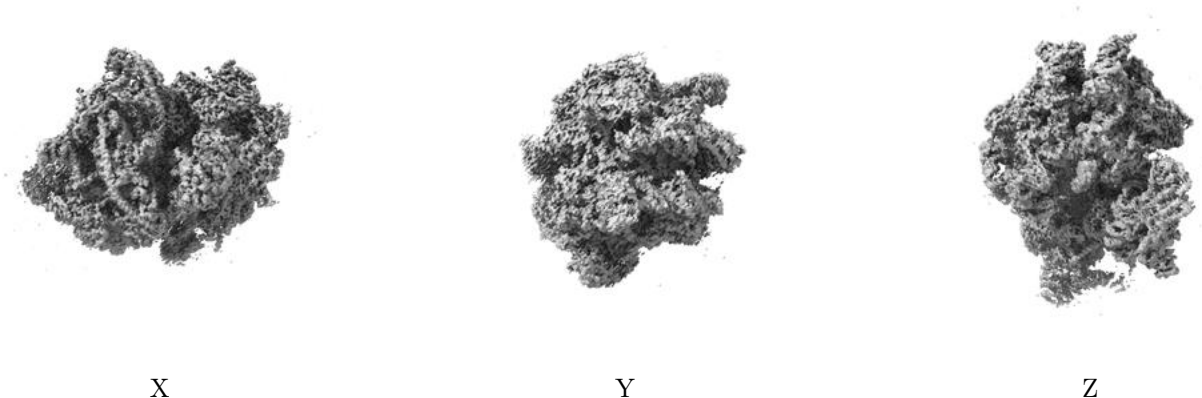


Z

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

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

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

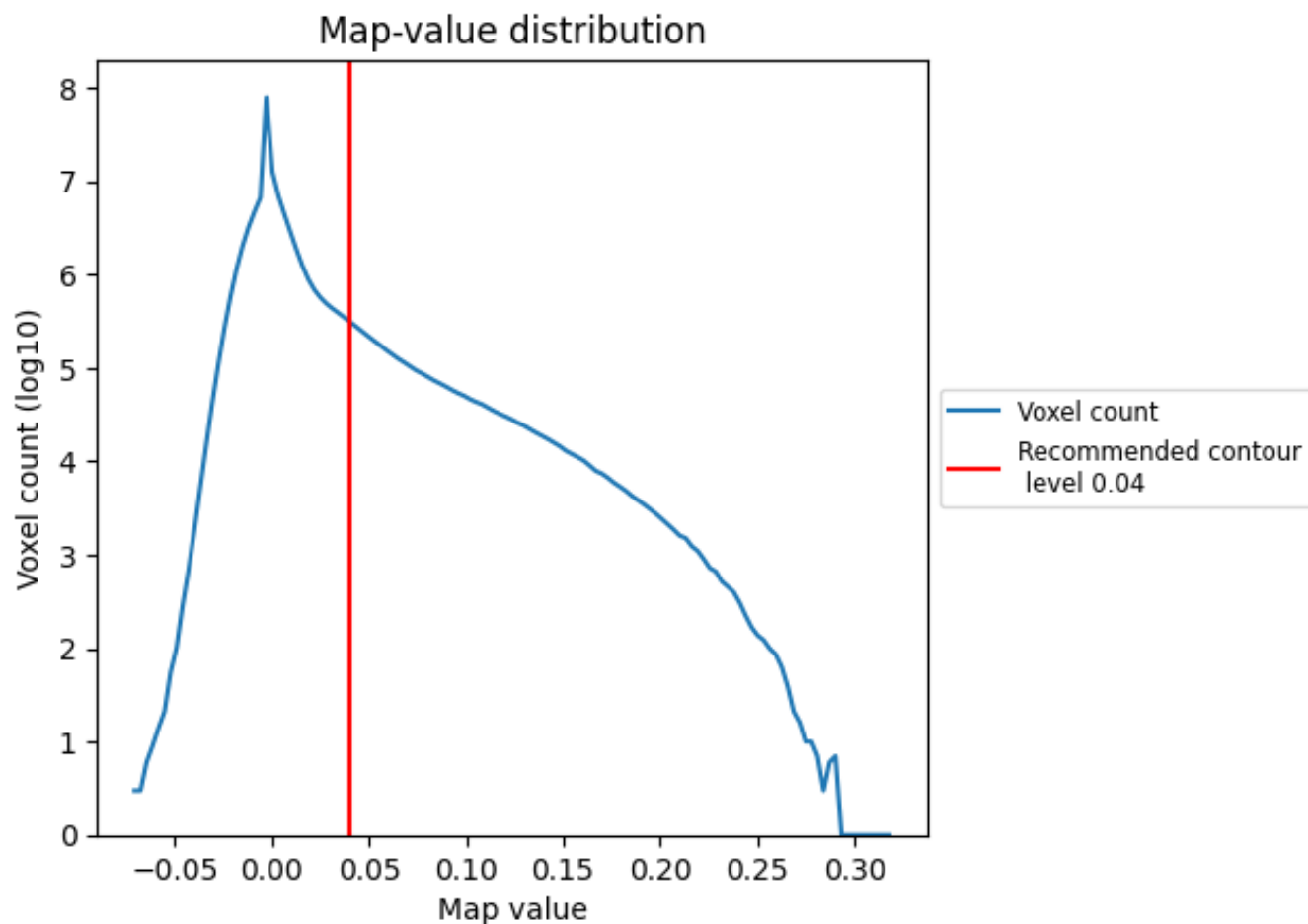
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

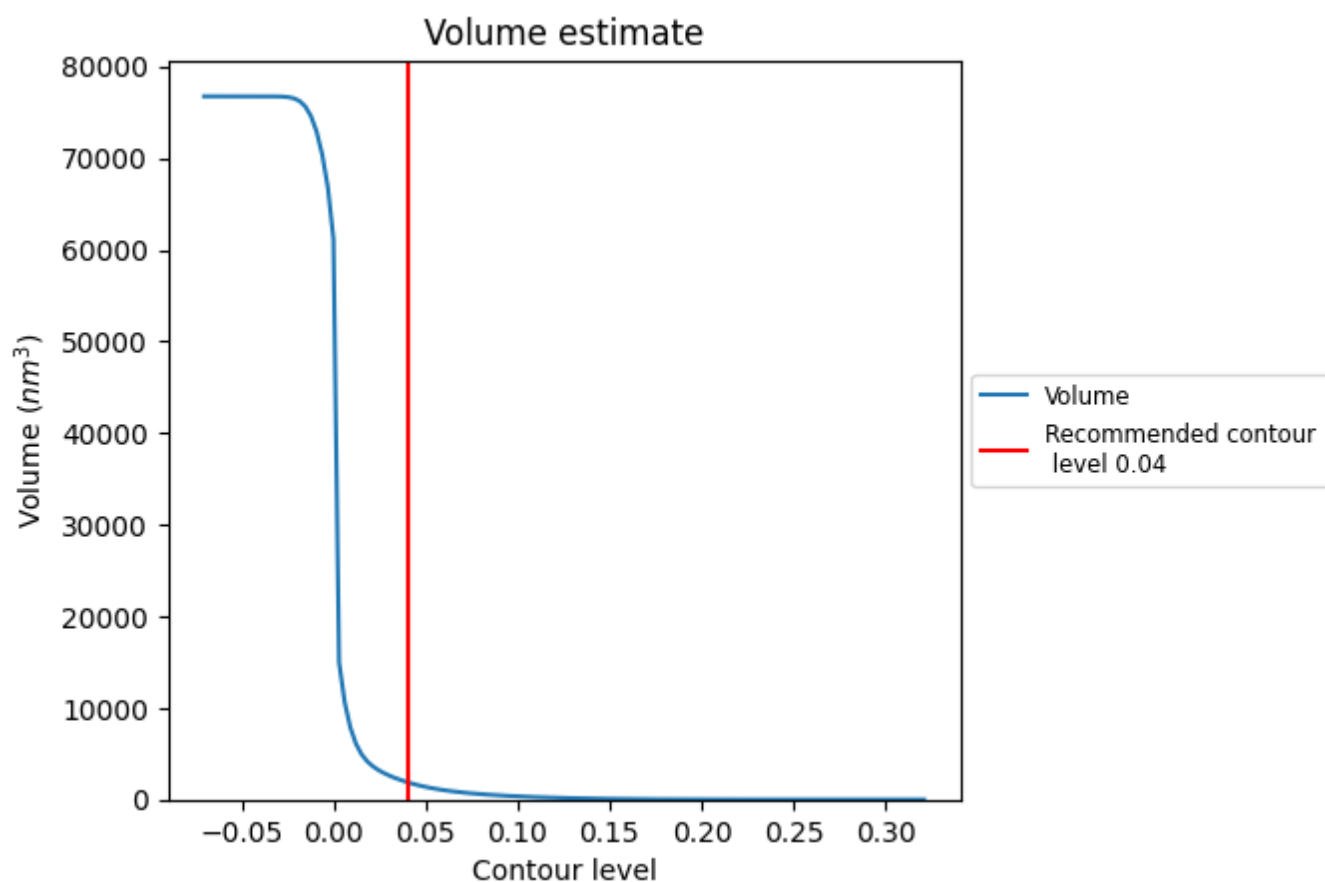
This section contains the results of statistical analysis of the map.

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



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

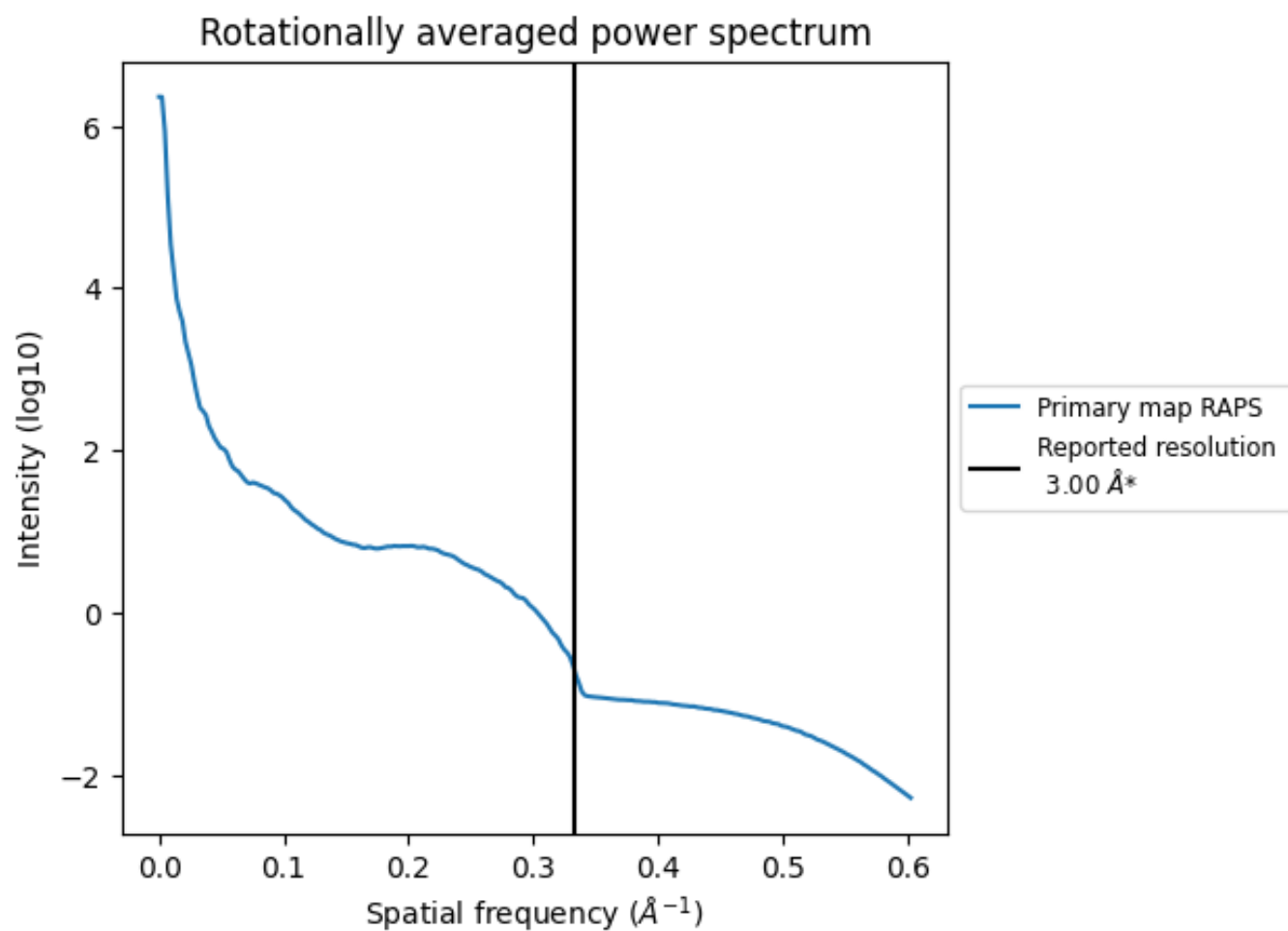
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1886 nm<sup>3</sup>; this corresponds to an approximate mass of 1704 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 0.333 Å<sup>-1</sup>

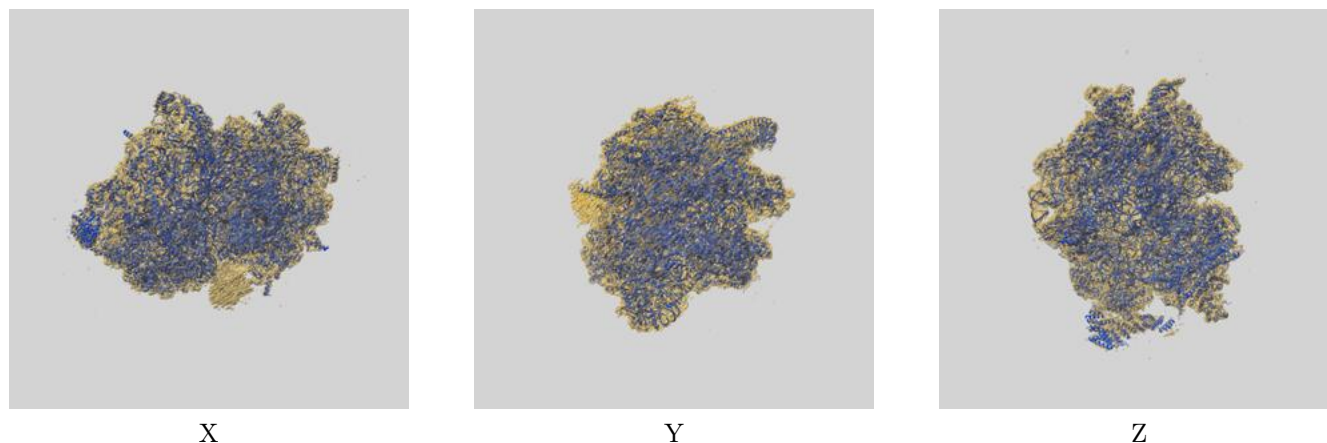
## 8 Fourier-Shell correlation

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

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

This section contains information regarding the fit between EMDB map EMD-64554 and PDB model 9UWH. Per-residue inclusion information can be found in section [3](#) on page [26](#).

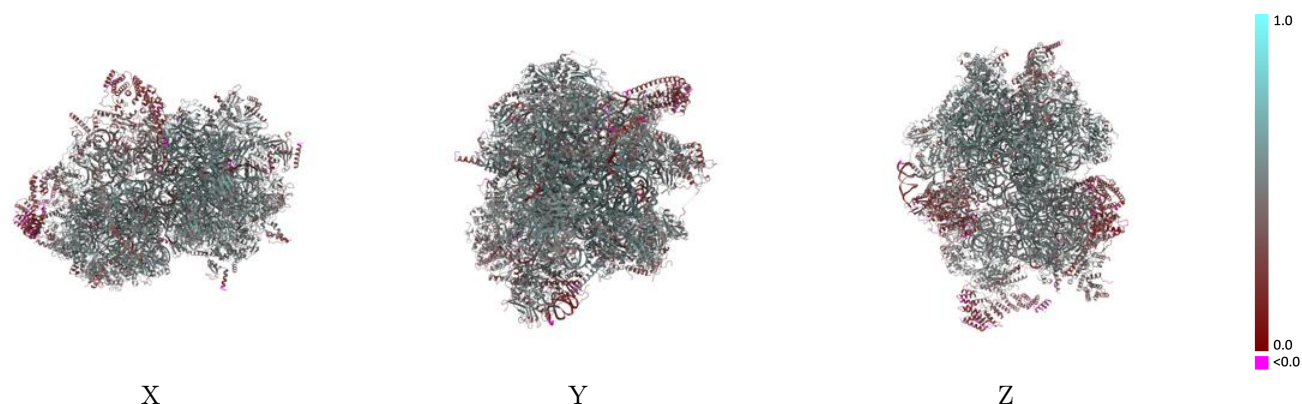
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.04 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.

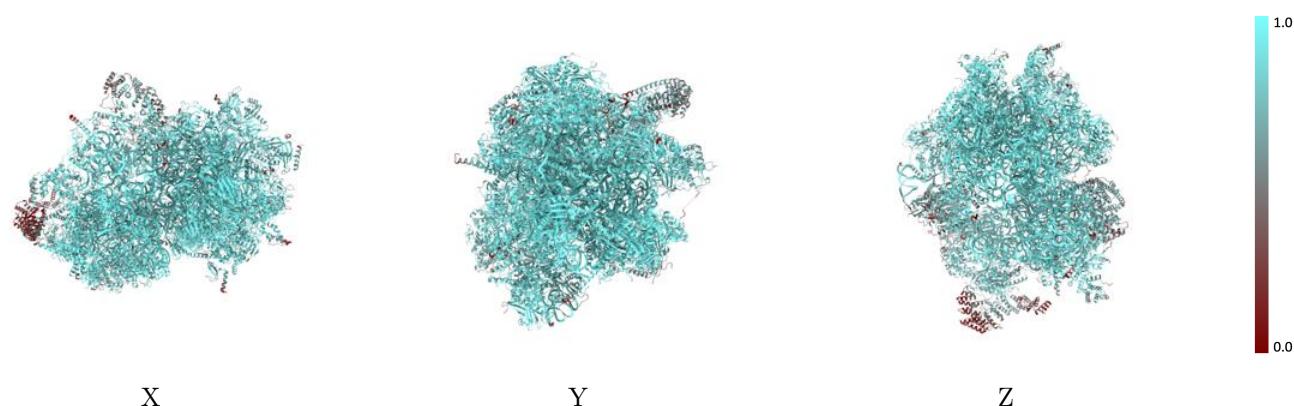


## 9.2 Q-score mapped to coordinate model [i](#)



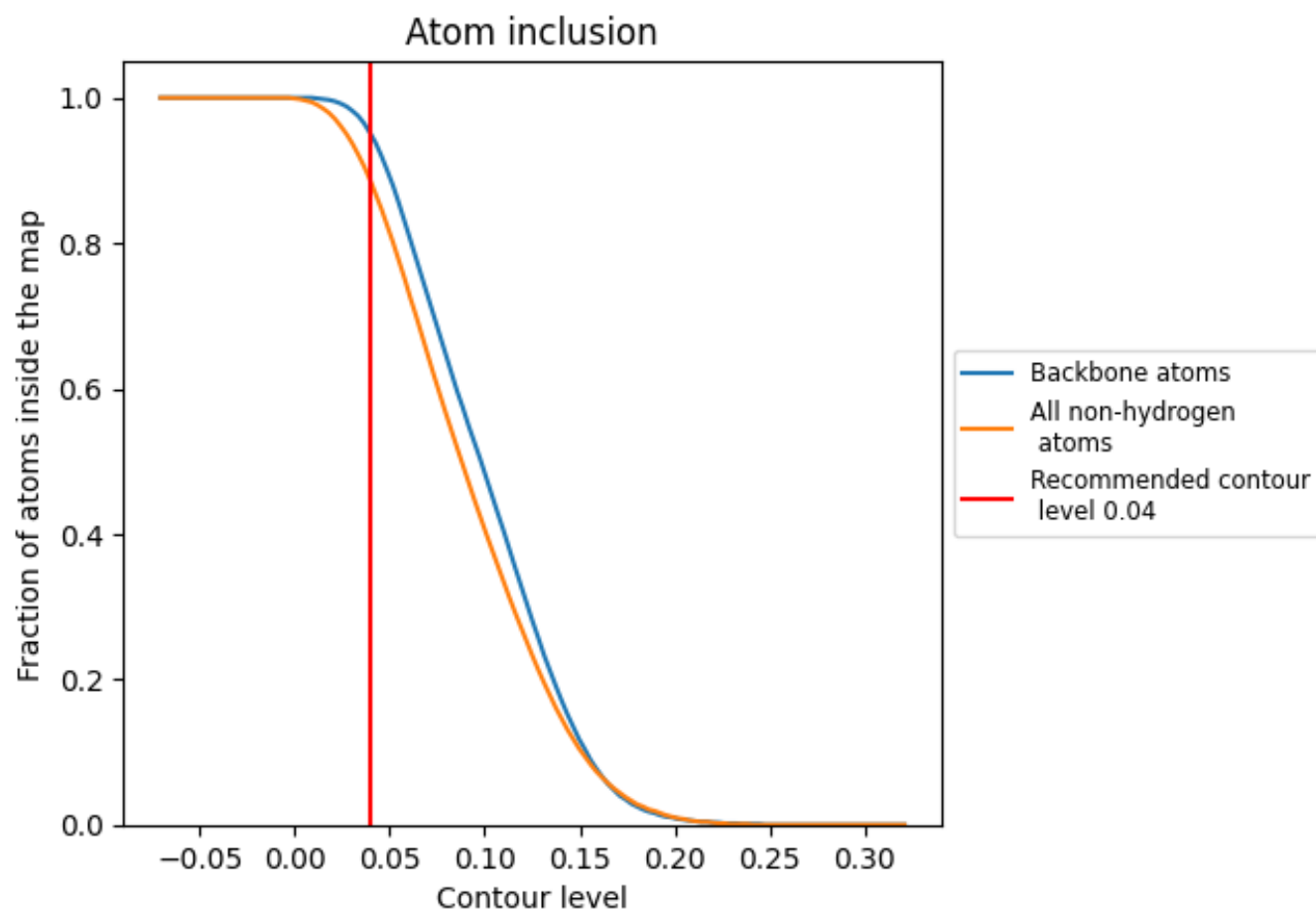
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.04).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 95% 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 (0.04) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.8850   |  0.4710   |
| 0     |  0.9130   |  0.5220   |
| 1     |  0.9390   |  0.5290   |
| 2     |  0.9950   |  0.5750   |
| 3     |  0.9830   |  0.5750   |
| 4     |  0.9630   |  0.5360   |
| 5     |  0.9120   |  0.5090   |
| 6     |  0.8890   |  0.4600   |
| 7     |  0.8380   |  0.4390   |
| 8     |  0.6930   |  0.3330   |
| 9     |  0.8590   |  0.4890   |
| A     |  0.9840   |  0.5220   |
| A0    |  0.7440   |  0.3630   |
| A1    |  0.7760   |  0.4220   |
| A2    |  0.8930  |  0.4710  |
| A3    |  0.9510 |  0.5140 |
| A4    |  0.3840 |  0.2300 |
| AA    |  0.9750 |  0.5010 |
| AB    |  0.9250 |  0.5080 |
| AC    |  0.8980 |  0.5060 |
| AD    |  0.8690 |  0.4840 |
| AE    |  0.9110 |  0.5110 |
| AF    |  0.8960 |  0.4600 |
| AG    |  0.8890 |  0.4680 |
| AH    |  0.8020 |  0.4500 |
| AI    |  0.9280 |  0.5200 |
| AJ    |  0.8580 |  0.4970 |
| AK    |  0.9180 |  0.5110 |
| AL    |  0.8720 |  0.4610 |
| AM    |  0.8330 |  0.4450 |
| AN    |  0.9380 |  0.5270 |
| AO    |  0.8300 |  0.4260 |
| AP    |  0.9300 |  0.5160 |
| AQ    |  0.9600 |  0.5350 |
| AR    |  0.8000 |  0.4000 |



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| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| AS    |  0.8130   |  0.4450   |
| AT    |  0.8970   |  0.4800   |
| AU    |  0.7840   |  0.4010   |
| AV    |  0.5680   |  0.2350   |
| AW    |  0.9090   |  0.4910   |
| AX    |  0.8420   |  0.4410   |
| AY    |  0.7300   |  0.3870   |
| AZ    |  0.8270   |  0.4580   |
| Ax    |  0.9190   |  0.3980   |
| Az    |  0.9640   |  0.4310   |
| B     |  0.8860   |  0.3270   |
| D     |  0.9630   |  0.5520   |
| E     |  0.9410   |  0.5260   |
| F     |  0.9600   |  0.5390   |
| H     |  0.7680   |  0.4240   |
| I     |  0.6510   |  0.3370   |
| J     |  0.6600   |  0.2330   |
| K     |  0.9560  |  0.5300  |
| L     |  0.9070 |  0.5240 |
| M     |  0.9400 |  0.5310 |
| N     |  0.9200 |  0.5100 |
| O     |  0.9100 |  0.5130 |
| P     |  0.9190 |  0.4990 |
| Q     |  0.8410 |  0.4960 |
| R     |  0.9580 |  0.5450 |
| S     |  0.9290 |  0.5290 |
| T     |  0.9510 |  0.5470 |
| U     |  0.8750 |  0.4760 |
| V     |  0.8330 |  0.4480 |
| W     |  0.9340 |  0.5430 |
| X     |  0.8840 |  0.4920 |
| Y     |  0.9280 |  0.5120 |
| Z     |  0.9280 |  0.5360 |
| a     |  0.8240 |  0.4500 |
| b     |  0.9390 |  0.5380 |
| c     |  0.8880 |  0.4800 |
| d     |  0.7980 |  0.4060 |
| e     |  0.6400 |  0.2670 |
| f     |  0.7210 |  0.3980 |
| g     |  0.9180 |  0.5160 |
| h     |  0.8560 |  0.4380 |
| i     |  0.9710 |  0.5660 |

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| Chain | Atom inclusion                                                                           | Q-score                                                                                  |
|-------|------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------|
| j     |  0.8410 |  0.4670 |
| k     |  0.7410 |  0.3440 |
| l     |  0.6820 |  0.2940 |
| m     |  0.6660 |  0.3170 |
| o     |  0.9630 |  0.5300 |
| p     |  0.7720 |  0.4120 |
| q     |  0.8010 |  0.4080 |
| r     |  0.9000 |  0.4930 |
| s     |  0.9340 |  0.5140 |
| t     |  0.2360 |  0.2580 |