



## Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 11:44 AM UTC

PDB ID : 7QP6 / pdb\_00007qp6  
EMDB ID : EMD-14113  
Title : Structure of the human 48S initiation complex in open state (h48S AUG open)  
Authors : Yi, S.-H.; Petrychenko, V.; Schliep, J.E.; Goyal, A.; Linden, A.; Chari, A.;  
Urlaub, H.; Stark, H.; Rodnina, M.V.; Adio, S.; Fischer, N.  
Deposited on : 2022-01-03  
Resolution : 4.70 Å(reported)  
Based on initial model : 6ZMW

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:

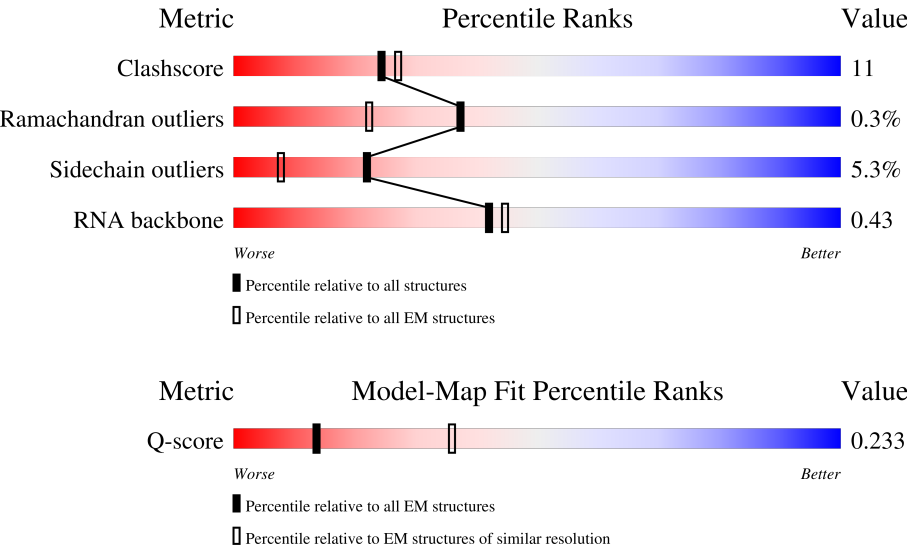
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 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 4.70 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                       | 1989 ( 4.20 - 5.20 )                                     |

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   | 1     | 813    | <div> <div>15%</div> <div>39%</div> <div>12%</div> <div>48%</div> </div> |
| 2   | 3     | 218    | <div> <div>49%</div> <div>88%</div> <div>10%</div> </div>                |
| 3   | 4     | 357    | <div> <div>13%</div> <div>65%</div> <div>7%</div> <div>28%</div> </div>  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 4   | 5     | 564    |                  |
| 5   | 6     | 374    |                  |
| 6   | 7     | 20     |                  |
| 7   | 8     | 352    |                  |
| 8   | 9     | 25     |                  |
| 9   | A     | 1869   |                  |
| 10  | B     | 158    |                  |
| 11  | C     | 263    |                  |
| 12  | D     | 194    |                  |
| 13  | E     | 143    |                  |
| 14  | F     | 59     |                  |
| 15  | G     | 194    |                  |
| 16  | H     | 84     |                  |
| 17  | I     | 151    |                  |
| 18  | J     | 130    |                  |
| 19  | K     | 83     |                  |
| 20  | L     | 293    |                  |
| 21  | M     | 135    |                  |
| 22  | N     | 295    |                  |
| 23  | O     | 264    |                  |
| 24  | P     | 151    |                  |
| 25  | Q     | 115    |                  |
| 26  | R     | 208    |                  |
| 27  | S     | 249    |                  |
| 28  | T     | 133    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 29  | V     | 204    |                  |
| 30  | Y     | 146    |                  |
| 31  | Z     | 243    |                  |
| 32  | a     | 165    |                  |
| 33  | b     | 145    |                  |
| 34  | c     | 317    |                  |
| 35  | d     | 145    |                  |
| 36  | e     | 125    |                  |
| 37  | f     | 152    |                  |
| 38  | h     | 119    |                  |
| 39  | i     | 56     |                  |
| 40  | k     | 156    |                  |
| 41  | m     | 132    |                  |
| 42  | n     | 69     |                  |
| 43  | o     | 320    |                  |
| 44  | p     | 113    |                  |
| 45  | q     | 144    |                  |
| 46  | r     | 315    |                  |
| 47  | s     | 333    |                  |
| 48  | t     | 472    |                  |
| 49  | u     | 1382   |                  |
| 50  | v     | 445    |                  |
| 51  | w     | 75     |                  |
| 52  | x     | 548    |                  |
| 53  | y     | 913    |                  |

## 2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 109900 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Eukaryotic translation initiation factor 3 subunit B.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 1   | 1     | 424      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2445  | 1501 | 469 | 470 | 5 |         |       |

- Molecule 2 is a protein called Eukaryotic translation initiation factor 3 subunit K.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 2   | 3     | 213      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1057  | 631 | 213 | 213 |         |       |

- Molecule 3 is a protein called Eukaryotic translation initiation factor 3 subunit F.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 3   | 4     | 257      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1272  | 757 | 257 | 258 |         |       |

- Molecule 4 is a protein called Eukaryotic translation initiation factor 3 subunit L.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 4   | 5     | 319      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1581  | 943 | 319 | 319 |         |       |

- Molecule 5 is a protein called Eukaryotic translation initiation factor 3 subunit M.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 5   | 6     | 350      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1917  | 1159 | 376 | 380 | 2 |         |       |

- Molecule 6 is a RNA chain called mRNA.

| Mol | Chain | Residues | Atoms |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---------|-------|
| 6   | 7     | 20       | Total | C   | O   | P  | 0       | 0     |
|     |       |          | 240   | 100 | 120 | 20 |         |       |

- Molecule 7 is a protein called Eukaryotic translation initiation factor 3 subunit H.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 7   | 8     | 317      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1571  | 936 | 317 | 318 |         |       |

- Molecule 8 is a protein called 60S ribosomal protein L41.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 8   | 9     | 24       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 230   | 139 | 62 | 26 | 3 |         |       |

- Molecule 9 is a RNA chain called 18S rRNA.

| Mol | Chain | Residues | Atoms |       |      |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|-------|
| 9   | A     | 1719     | Total | C     | N    | O     | P    | 0       | 0     |
|     |       |          | 36668 | 16378 | 6574 | 11998 | 1718 |         |       |

- Molecule 10 is a protein called 40S ribosomal protein S11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 10  | B     | 142      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1166  | 743 | 218 | 199 | 6 |         |       |

- Molecule 11 is a protein called 40S ribosomal protein S4, X isoform.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 11  | C     | 256      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2035  | 1302 | 378 | 347 | 8 |         |       |

- Molecule 12 is a protein called 40S ribosomal protein S9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 12  | D     | 177      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1477  | 941 | 295 | 239 | 2 |         |       |

- Molecule 13 is a protein called 40S ribosomal protein S23.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 13  | E     | 140      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1087  | 687 | 215 | 182 | 3 |         |       |

- Molecule 14 is a protein called 40S ribosomal protein S30.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 14  | F     | 40       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 330   | 204 | 75 | 50 | 1 |         |       |

- Molecule 15 is a protein called 40S ribosomal protein S7.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 15  | G     | 177      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1430  | 917 | 260 | 252 | 1 |         |       |

- Molecule 16 is a protein called 40S ribosomal protein S27.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 16  | H     | 81       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 631   | 397 | 116 | 111 | 7 |         |       |

- Molecule 17 is a protein called 40S ribosomal protein S13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 17  | I     | 150      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1208  | 773 | 229 | 205 | 1 |         |       |

- Molecule 18 is a protein called 40S ribosomal protein S15a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 18  | J     | 129      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1034  | 659 | 193 | 176 | 6 |         |       |

- Molecule 19 is a protein called 40S ribosomal protein S21.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19  | K     | 81       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 617   | 380 | 114 | 118 | 5 |         |       |

- Molecule 20 is a protein called 40S ribosomal protein S2.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 20  | L     | 220      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1707  | 1104 | 292 | 301 | 10 |         |       |

- Molecule 21 is a protein called 40S ribosomal protein S17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 21  | M     | 131      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1064  | 668 | 198 | 194 | 4 |         |       |

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

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 22  | N     | 207      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1633  | 1040 | 288 | 297 | 8 |         |       |

- Molecule 23 is a protein called 40S ribosomal protein S3a.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 23  | O     | 211      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1715  | 1088 | 307 | 306 | 14 |         |       |

- Molecule 24 is a protein called 40S ribosomal protein S14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 24  | P     | 133      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 997   | 610 | 196 | 185 | 6 |         |       |

- Molecule 25 is a protein called 40S ribosomal protein S26.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 25  | Q     | 99       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 792   | 492 | 165 | 130 | 5 |         |       |

- Molecule 26 is a protein called 40S ribosomal protein S8.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 26  | R     | 198      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1627  | 1021 | 322 | 279 | 5 |         |       |

- Molecule 27 is a protein called 40S ribosomal protein S6.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 27  | S     | 230      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1862  | 1164 | 371 | 320 | 7 |         |       |

- Molecule 28 is a protein called 40S ribosomal protein S24.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 28  | T     | 125      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1015  | 642 | 199 | 169 | 5 |         |       |

- Molecule 29 is a protein called 40S ribosomal protein S5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 29  | V     | 184      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1461  | 914 | 276 | 264 | 7 |         |       |

- Molecule 30 is a protein called 40S ribosomal protein S16.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 30  | Y     | 141      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1124  | 715 | 212 | 194 | 3 |         |       |

- Molecule 31 is a protein called 40S ribosomal protein S3.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 31  | Z     | 227      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1765  | 1125 | 317 | 315 | 8 |         |       |

- Molecule 32 is a protein called 40S ribosomal protein S10.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 32  | a     | 99       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 834   | 544 | 149 | 135 | 6 |         |       |

- Molecule 33 is a protein called 40S ribosomal protein S15.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 33  | b     | 110      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 913   | 580 | 168 | 158 | 7 |         |       |

- Molecule 34 is a protein called Receptor of activated protein C kinase 1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 34  | c     | 313      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2436  | 1535 | 424 | 465 | 12 |         |       |

- Molecule 35 is a protein called 40S ribosomal protein S19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 35  | d     | 142      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1105  | 692 | 213 | 197 | 3 |         |       |

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

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 36  | e     | 66       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 523   | 338 | 93 | 91 | 1 |         |       |

- Molecule 37 is a protein called 40S ribosomal protein S18.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 37  | f     | 142      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1176  | 737 | 239 | 199 | 1 |         |       |

- Molecule 38 is a protein called 40S ribosomal protein S20.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 38  | h     | 103      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 817   | 511 | 155 | 147 | 4 |         |       |

- Molecule 39 is a protein called 40S ribosomal protein S29.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 39  | i     | 50       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 419   | 262 | 85 | 67 | 5 |         |       |

- Molecule 40 is a protein called Ubiquitin-40S ribosomal protein S27a.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 40  | k     | 53       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 435   | 276 | 82 | 70 | 7 |         |       |

- Molecule 41 is a protein called 40S ribosomal protein S12.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 41  | m     | 122      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 950   | 596 | 168 | 177 | 9 |         |       |

- Molecule 42 is a protein called 40S ribosomal protein S28.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 42  | n     | 63       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 498   | 302 | 101 | 93 | 2 |         |       |

- Molecule 43 is a protein called Eukaryotic translation initiation factor 3 subunit G.

| Mol | Chain | Residues | Atoms |     |     |     |  | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|--|---------|-------|
| 43  | o     | 77       | Total | C   | N   | O   |  | 0       | 0     |
|     |       |          | 616   | 389 | 111 | 116 |  |         |       |

- Molecule 44 is a protein called Eukaryotic translation initiation factor 1.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 44  | p     | 85       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 691   | 438 | 125 | 126 | 2 |         |       |

- Molecule 45 is a protein called Eukaryotic translation initiation factor 1A, X-chromosomal.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 45  | q     | 88       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 714   | 451 | 129 | 130 | 4 |         |       |

- Molecule 46 is a protein called Eukaryotic translation initiation factor 2 subunit 1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 46  | r     | 275      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2215  | 1398 | 387 | 418 | 12 |         |       |

- Molecule 47 is a protein called Eukaryotic translation initiation factor 2 subunit 2.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 47  | s     | 138      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1123  | 709 | 206 | 199 | 9 |         |       |

- Molecule 48 is a protein called Eukaryotic translation initiation factor 2 subunit 3.

| Mol | Chain | Residues | Atoms |      |     |     |  | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|--|---------|-------|
| 48  | t     | 356      | Total | C    | N   | O   |  | 0       | 0     |
|     |       |          | 1750  | 1038 | 356 | 356 |  |         |       |

- Molecule 49 is a protein called Eukaryotic translation initiation factor 3 subunit A.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 49  | u     | 706      | Total | C    | N   | O   | S  | 1       | 0     |
|     |       |          | 5383  | 3379 | 982 | 999 | 23 |         |       |

- Molecule 50 is a protein called Eukaryotic translation initiation factor 3 subunit E.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 50  | v     | 384      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2635  | 1657 | 477 | 489 | 12 |         |       |

- Molecule 51 is a RNA chain called Initiator Met-tRNA-i.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 51  | w     | 75       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1604  | 717 | 298 | 515 | 74 |         |       |

- Molecule 52 is a protein called Eukaryotic translation initiation factor 3 subunit D.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 52  | x     | 421      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2831  | 1746 | 521 | 555 | 9 |         |       |

- Molecule 53 is a protein called Eukaryotic translation initiation factor 3 subunit C.

| Mol | Chain | Residues | Atoms |      |     |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|----|---------|-------|
| 53  | y     | 697      | Total | C    | N   | O    | S  | 0       | 0     |
|     |       |          | 5470  | 3437 | 980 | 1018 | 35 |         |       |

- Molecule 54 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 54  | Q     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 54  | k     | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |

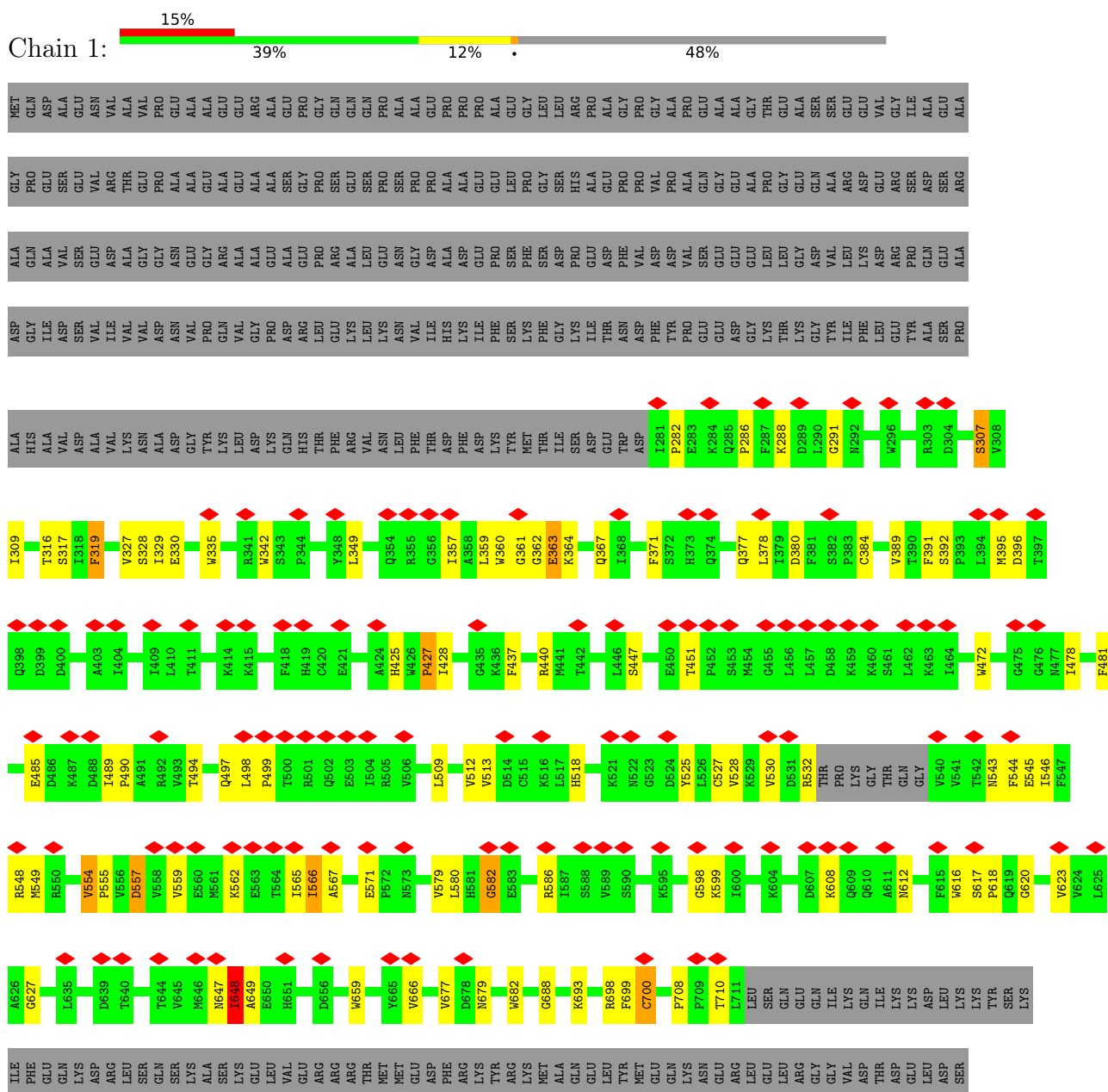
- Molecule 55 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 55  | d     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |
| 55  | f     | 1        | Total | Mg | 0       |
|     |       |          | 1     | 1  |         |

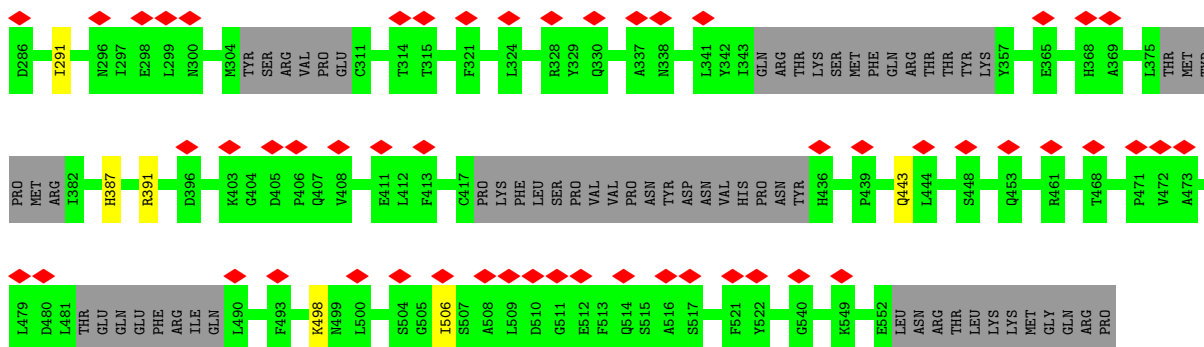
### 3 Residue-property plots

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

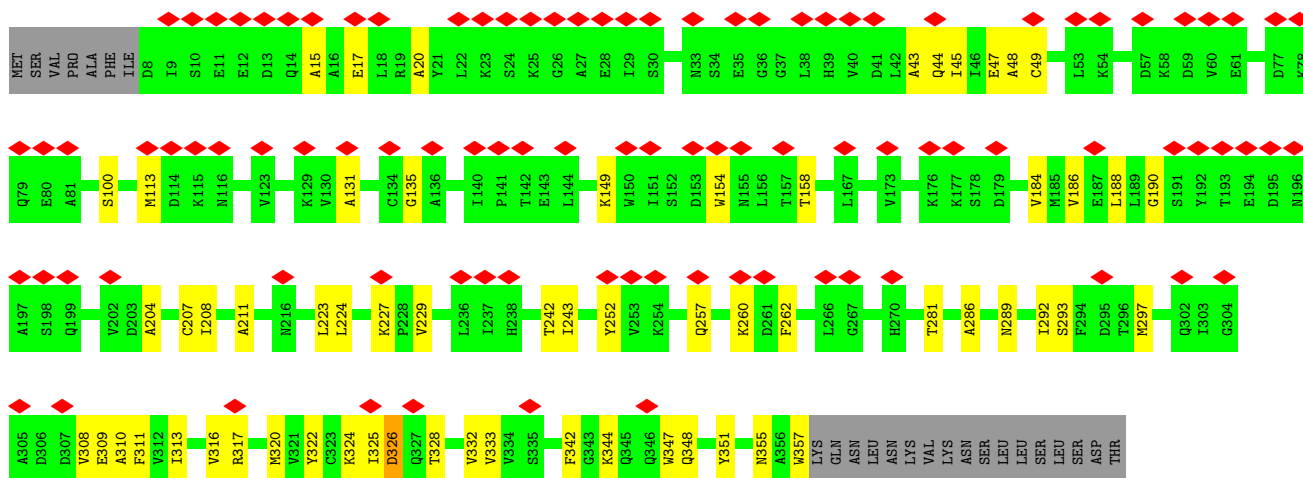
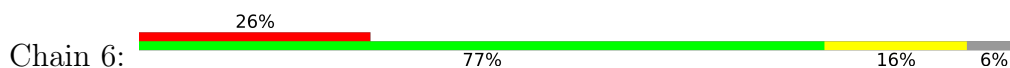
- Molecule 1: Eukaryotic translation initiation factor 3 subunit B







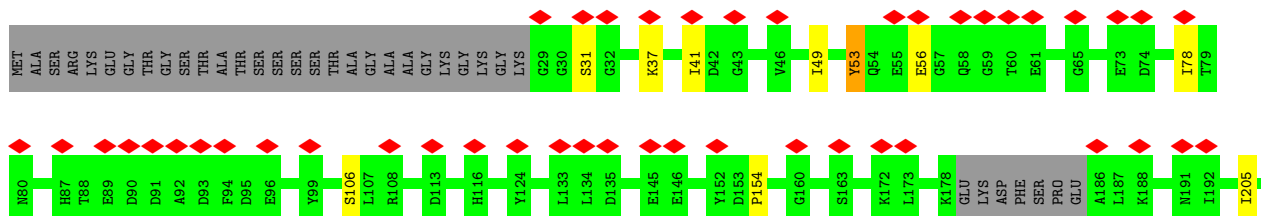
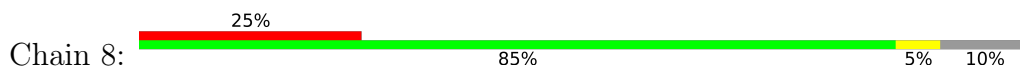
• Molecule 5: Eukaryotic translation initiation factor 3 subunit M



• Molecule 6: mRNA



• Molecule 7: Eukaryotic translation initiation factor 3 subunit H



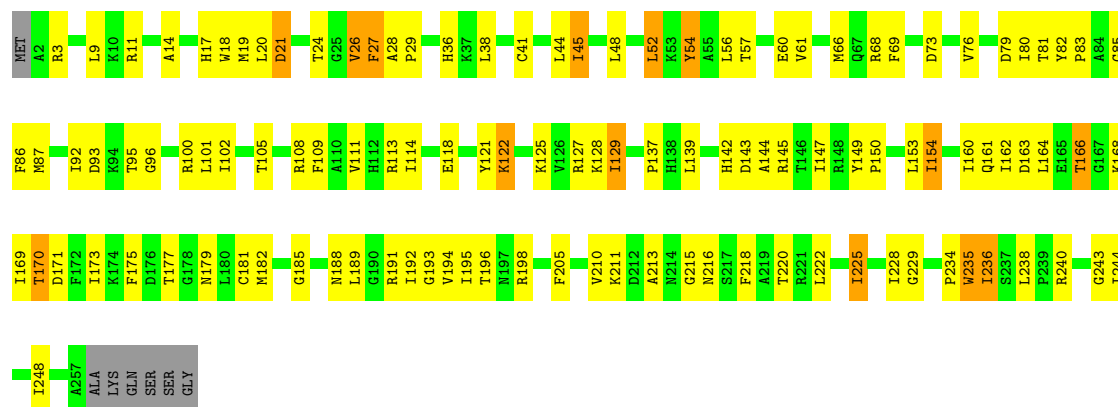






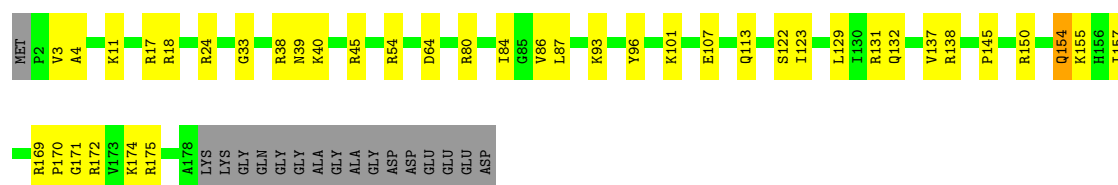
- Molecule 11: 40S ribosomal protein S4, X isoform

Chain C: 53% 39% 5%



- Molecule 12: 40S ribosomal protein S9

Chain D: 71% 20% 9%



- Molecule 13: 40S ribosomal protein S23

Chain E: 79% 19%



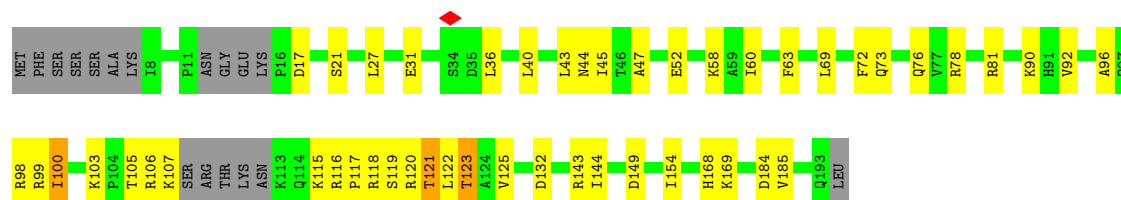
- Molecule 14: 40S ribosomal protein S30

Chain F: 37% 29% 32%



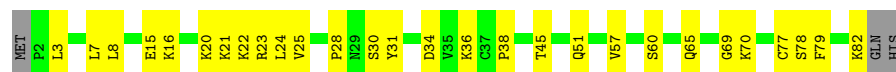
- Molecule 15: 40S ribosomal protein S7

Chain G: 66% 24% 9%



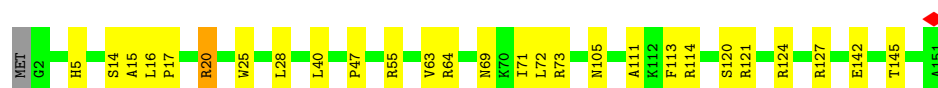
- Molecule 16: 40S ribosomal protein S27

Chain H: 63% 33% .



- Molecule 17: 40S ribosomal protein S13

Chain I: 81% 17% ..



- Molecule 18: 40S ribosomal protein S15a

Chain J: 81% 16% ..



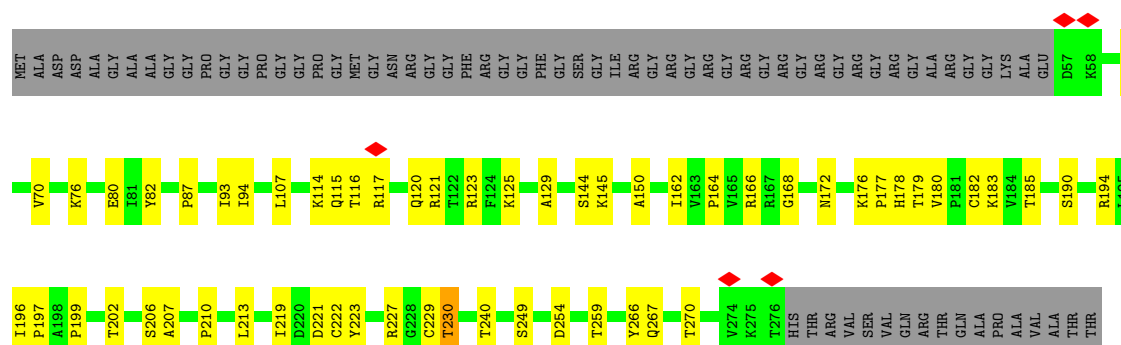
- Molecule 19: 40S ribosomal protein S21

Chain K: 76% 22% .

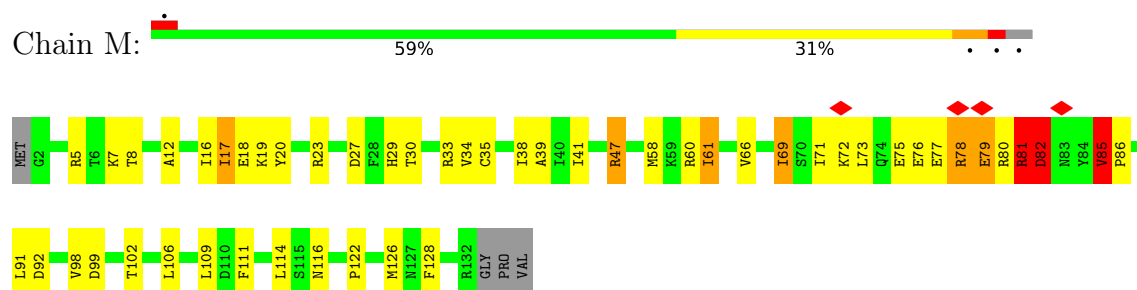


- Molecule 20: 40S ribosomal protein S2

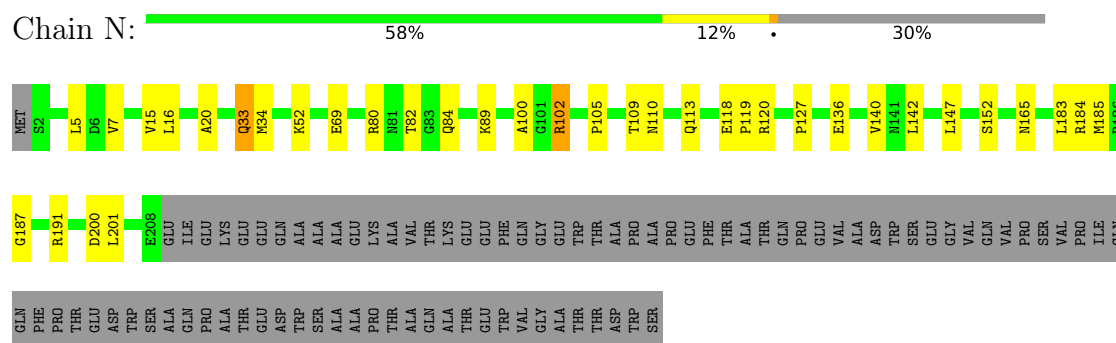
Chain L: 55% 19% 25%



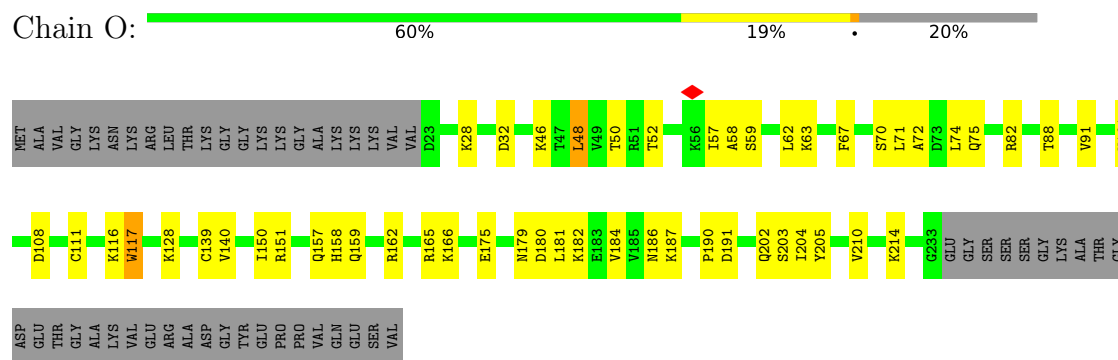
- Molecule 21: 40S ribosomal protein S17



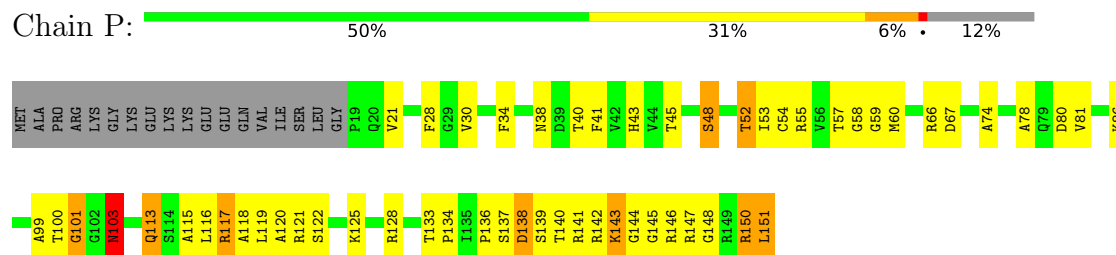
- Molecule 22: 40S ribosomal protein SA



- Molecule 23: 40S ribosomal protein S3a

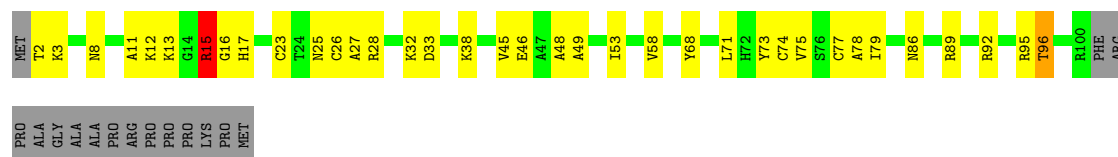


- Molecule 24: 40S ribosomal protein S14



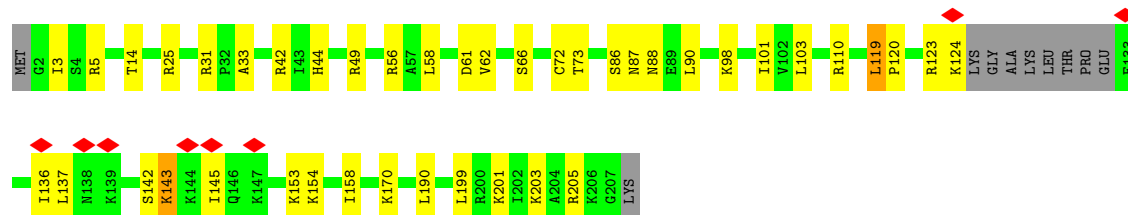
- Molecule 25: 40S ribosomal protein S26





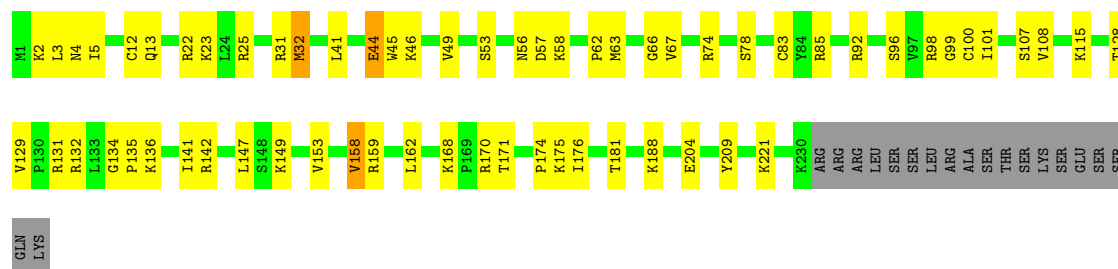
- Molecule 26: 40S ribosomal protein S8

Chain R: 75% 19% 5%



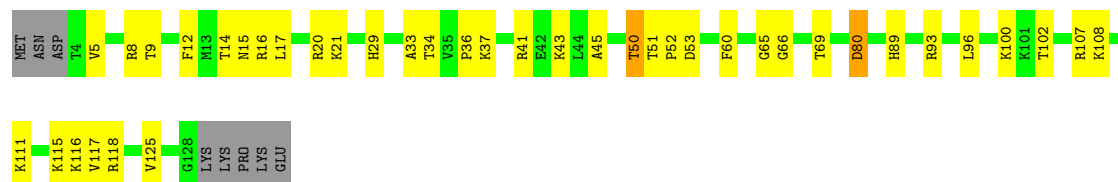
- Molecule 27: 40S ribosomal protein S6

Chain S: 67% 24% 8%



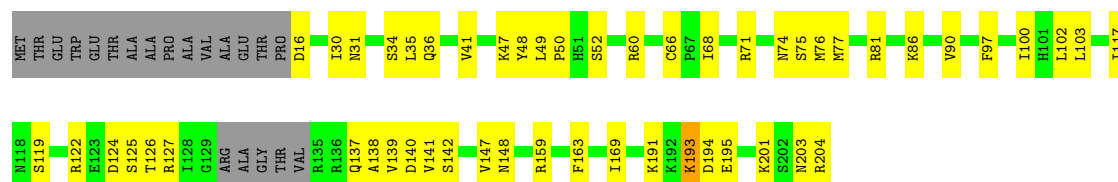
- Molecule 28: 40S ribosomal protein S24

Chain T: 64% 29% 6%



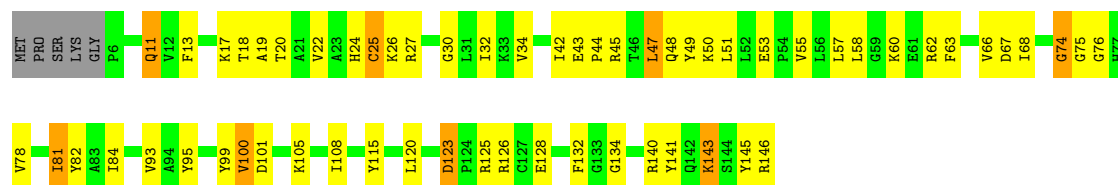
- Molecule 29: 40S ribosomal protein S5

Chain V: 65% 25% 10%



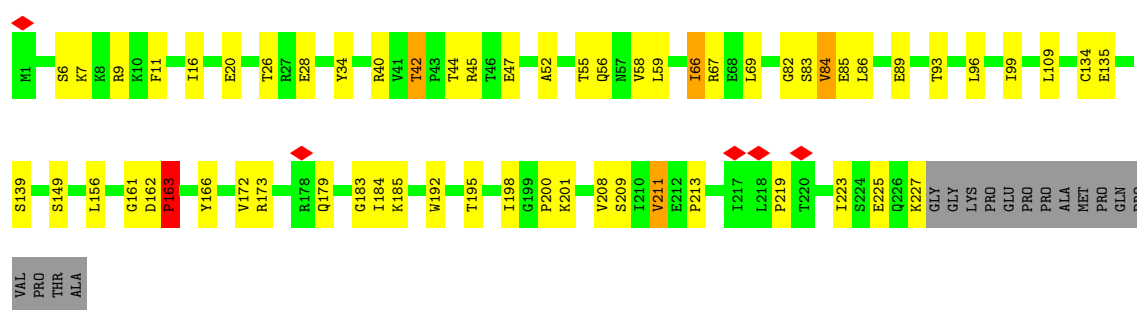
- Molecule 30: 40S ribosomal protein S16

Chain Y:  55% 36% 5% .

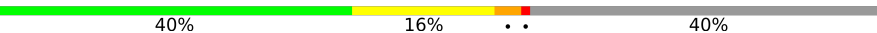


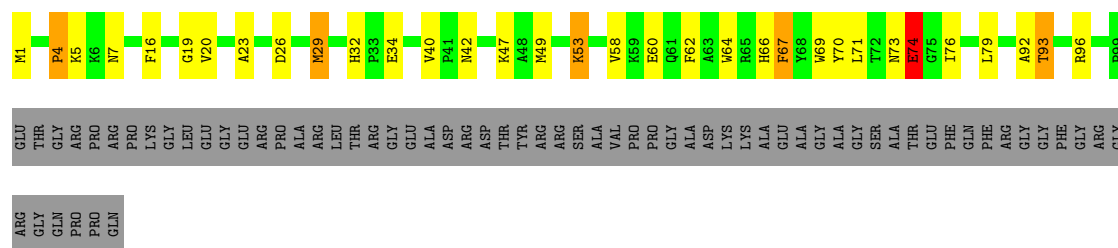
- Molecule 31: 40S ribosomal protein S3

Chain Z:  69% 23% 7% .



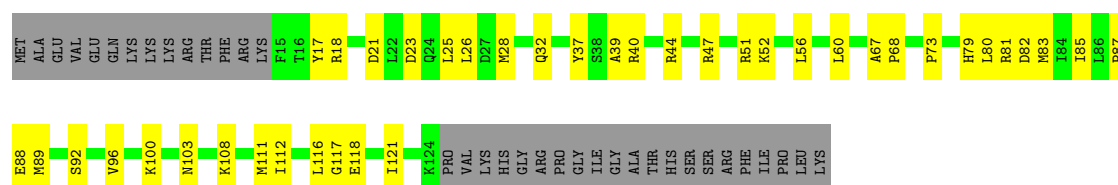
- Molecule 32: 40S ribosomal protein S10

Chain a:  40% 16% . . 40%



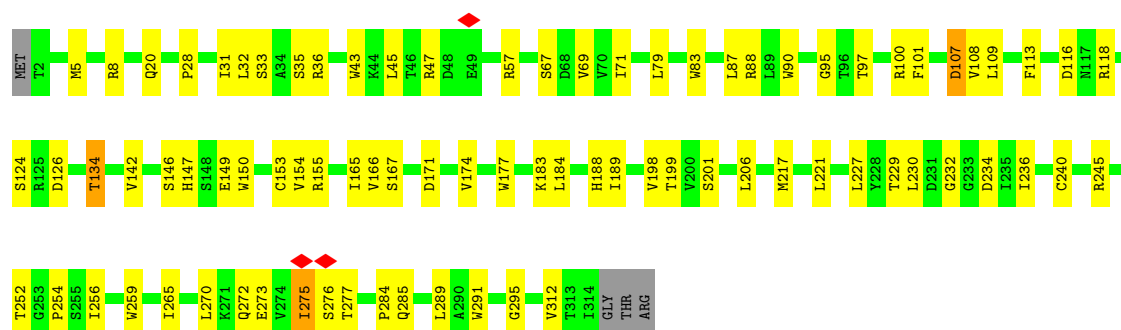
- Molecule 33: 40S ribosomal protein S15

Chain b:  48% 28% 24%

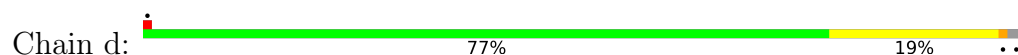


- Molecule 34: Receptor of activated protein C kinase 1

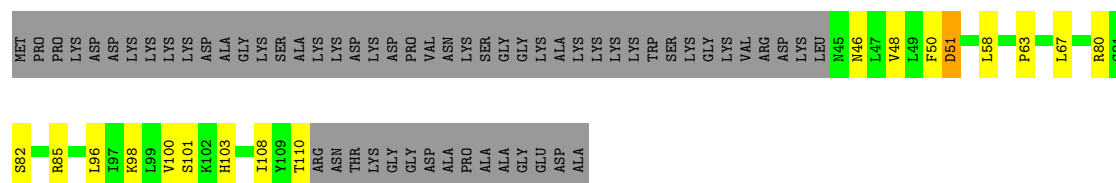
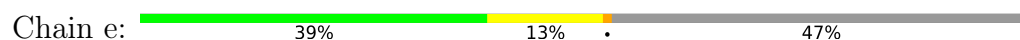
Chain c:  73% 25% ..



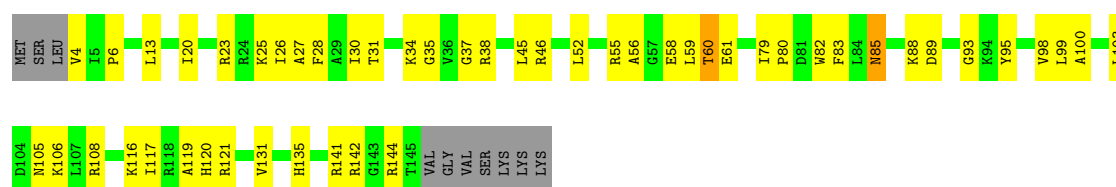
• Molecule 35: 40S ribosomal protein S19



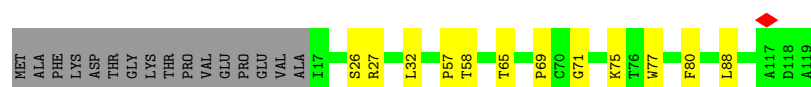
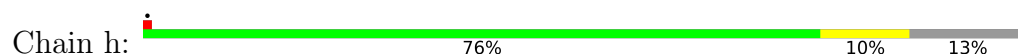
• Molecule 36: 40S ribosomal protein S25



• Molecule 37: 40S ribosomal protein S18



• Molecule 38: 40S ribosomal protein S20



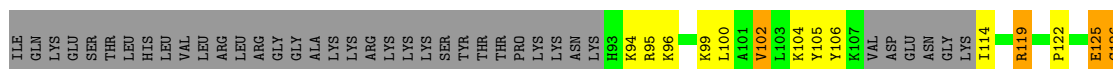
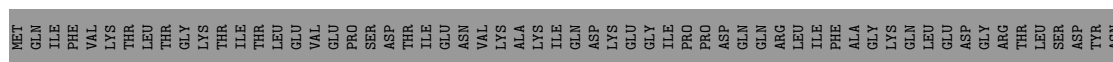
• Molecule 39: 40S ribosomal protein S29





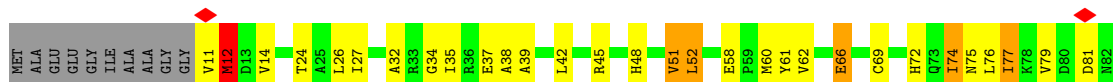
- Molecule 40: Ubiquitin-40S ribosomal protein S27a

Chain k: 14% 15% 5% 66%



- Molecule 41: 40S ribosomal protein S12

Chain m: 49% 33% 9% 8%



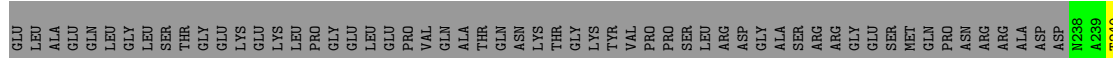
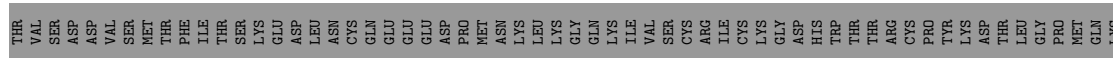
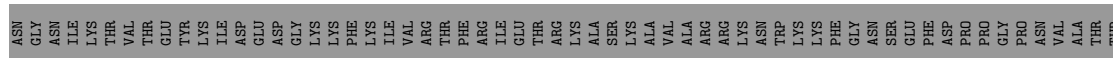
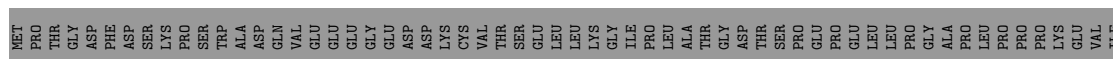
- Molecule 42: 40S ribosomal protein S28

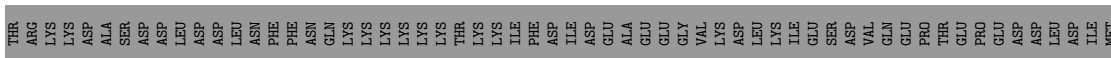
Chain n: 55% 35% 9%

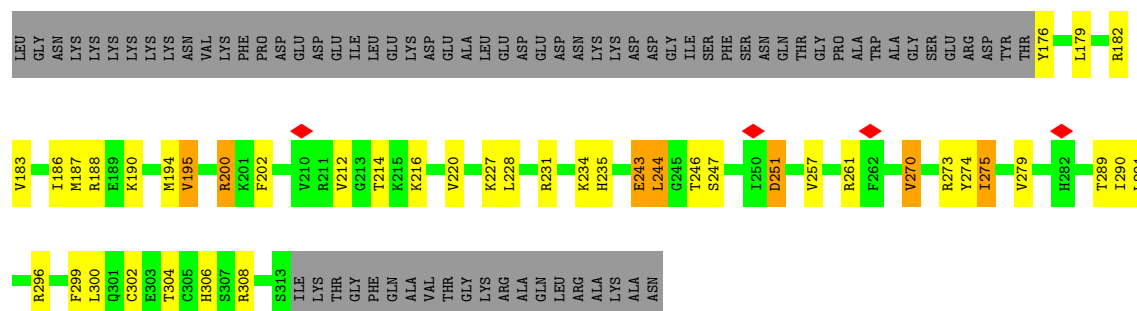


- Molecule 43: Eukaryotic translation initiation factor 3 subunit G

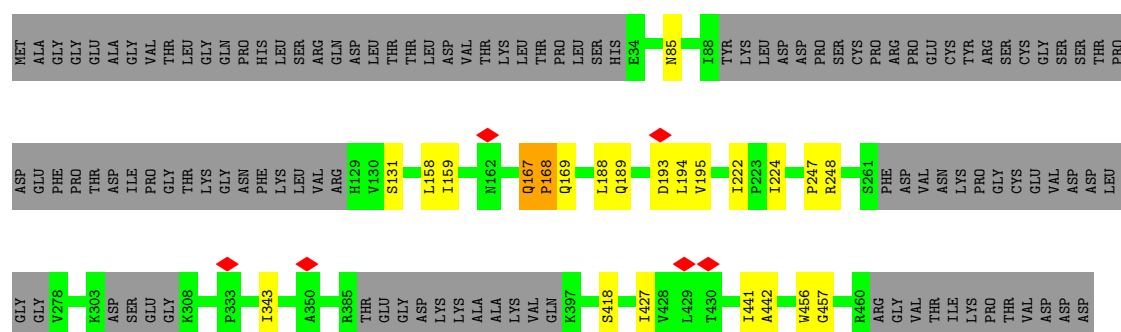
Chain o: 16% 8% 76%



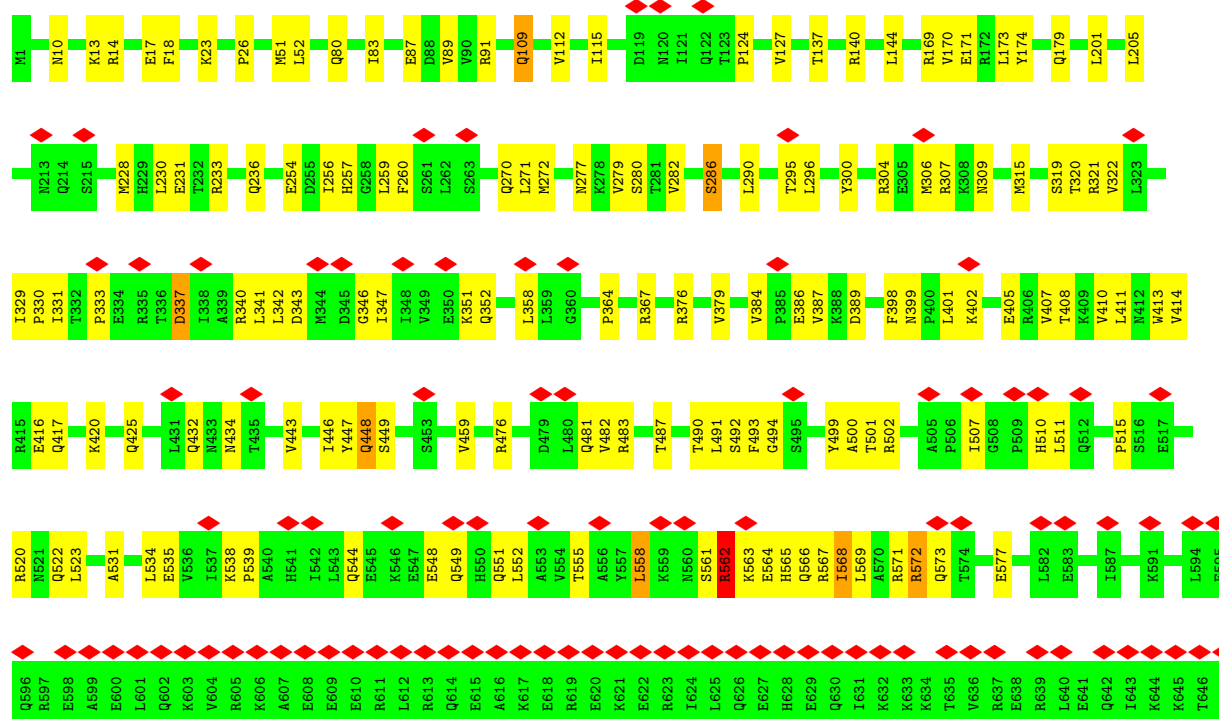
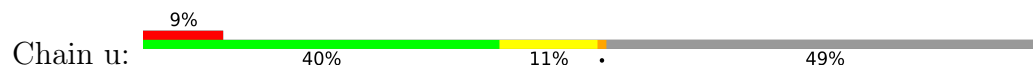




- Molecule 48: Eukaryotic translation initiation factor 2 subunit 3



- Molecule 49: Eukaryotic translation initiation factor 3 subunit A









## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, C1                               | Depositor |
| Number of particles used             | 57184                                   | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TITAN KRIOS                         | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 48                                      | Depositor |
| Minimum defocus (nm)                 | 1500                                    | Depositor |
| Maximum defocus (nm)                 | 4000                                    | Depositor |
| Magnification                        | 59000                                   | Depositor |
| Image detector                       | FEI FALCON III (4k x 4k)                | Depositor |
| Maximum map value                    | 20.695                                  | Depositor |
| Minimum map value                    | -7.349                                  | Depositor |
| Average map value                    | 0.000                                   | Depositor |
| Map value standard deviation         | 1.000                                   | Depositor |
| Recommended contour level            | 2.3                                     | Depositor |
| Map size (Å)                         | 417.59998, 417.59998, 417.59998         | wwPDB     |
| Map dimensions                       | 360, 360, 360                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.16, 1.16, 1.16                        | Depositor |

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PSU, MA6, UR3, A2M, OMG, OMU, ZN, 5MC, 5MU, MG, OMC

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   | 1     | 1.14         | 0/2466        | 1.82        | 53/3400 (1.6%)  |
| 2   | 3     | 1.02         | 0/1055        | 1.17        | 0/1469          |
| 3   | 4     | 1.08         | 0/1269        | 1.39        | 3/1762 (0.2%)   |
| 4   | 5     | 1.07         | 0/1575        | 1.24        | 0/2187          |
| 5   | 6     | 1.03         | 0/1926        | 1.39        | 13/2669 (0.5%)  |
| 6   | 7     | 0.53         | 0/259         | 1.14        | 2/396 (0.5%)    |
| 7   | 8     | 1.07         | 0/1569        | 1.37        | 4/2183 (0.2%)   |
| 8   | 9     | 0.64         | 0/231         | 1.51        | 1/294 (0.3%)    |
| 9   | A     | 0.47         | 0/40362       | 0.68        | 50/62905 (0.1%) |
| 10  | B     | 0.85         | 0/1186        | 1.36        | 5/1585 (0.3%)   |
| 11  | C     | 0.85         | 0/2077        | 1.38        | 3/2796 (0.1%)   |
| 12  | D     | 0.72         | 0/1502        | 0.93        | 1/2008 (0.0%)   |
| 13  | E     | 0.79         | 0/1105        | 1.16        | 1/1476 (0.1%)   |
| 14  | F     | 0.78         | 0/332         | 1.34        | 1/434 (0.2%)    |
| 15  | G     | 0.73         | 0/1451        | 1.13        | 1/1942 (0.1%)   |
| 16  | H     | 0.77         | 0/644         | 1.11        | 1/864 (0.1%)    |
| 17  | I     | 0.78         | 0/1232        | 1.13        | 0/1656          |
| 18  | J     | 0.77         | 0/1051        | 1.06        | 1/1406 (0.1%)   |
| 19  | K     | 0.82         | 0/623         | 1.09        | 0/833           |
| 20  | L     | 0.78         | 0/1743        | 1.12        | 0/2354          |
| 21  | M     | 0.85         | 0/1078        | 1.53        | 7/1447 (0.5%)   |
| 22  | N     | 0.76         | 0/1670        | 1.04        | 2/2271 (0.1%)   |
| 23  | O     | 0.74         | 0/1742        | 1.07        | 1/2330 (0.0%)   |
| 24  | P     | 1.22         | 3/1010 (0.3%) | 1.84        | 18/1353 (1.3%)  |
| 25  | Q     | 0.84         | 0/805         | 1.24        | 1/1079 (0.1%)   |
| 26  | R     | 0.72         | 0/1654        | 0.98        | 0/2203          |
| 27  | S     | 0.75         | 0/1885        | 1.04        | 1/2510 (0.0%)   |
| 28  | T     | 0.72         | 0/1032        | 1.00        | 0/1371          |
| 29  | V     | 0.83         | 0/1481        | 1.15        | 6/1988 (0.3%)   |
| 30  | Y     | 0.83         | 0/1142        | 1.38        | 2/1528 (0.1%)   |
| 31  | Z     | 0.82         | 0/1793        | 1.17        | 6/2414 (0.2%)   |
| 32  | a     | 0.83         | 0/859         | 1.34        | 3/1159 (0.3%)   |

| Mol | Chain | Bond lengths |                 | Bond angles |                   |
|-----|-------|--------------|-----------------|-------------|-------------------|
|     |       | RMSZ         | # Z  >5         | RMSZ        | # Z  >5           |
| 33  | b     | 0.73         | 0/929           | 0.98        | 0/1241            |
| 34  | c     | 0.76         | 0/2493          | 1.03        | 1/3394 (0.0%)     |
| 35  | d     | 0.76         | 0/1123          | 1.03        | 0/1504            |
| 36  | e     | 0.80         | 0/529           | 1.04        | 0/712             |
| 37  | f     | 0.74         | 0/1194          | 1.05        | 1/1599 (0.1%)     |
| 38  | h     | 0.78         | 0/827           | 1.07        | 0/1110            |
| 39  | i     | 0.79         | 0/429           | 1.51        | 3/568 (0.5%)      |
| 40  | k     | 0.87         | 0/444           | 1.52        | 3/588 (0.5%)      |
| 41  | m     | 0.92         | 0/960           | 1.48        | 8/1286 (0.6%)     |
| 42  | n     | 0.78         | 0/500           | 1.13        | 0/669             |
| 43  | o     | 0.82         | 0/628           | 1.08        | 1/846 (0.1%)      |
| 44  | p     | 0.85         | 0/701           | 1.70        | 7/936 (0.7%)      |
| 45  | q     | 0.88         | 0/722           | 1.49        | 6/963 (0.6%)      |
| 46  | r     | 0.44         | 1/2247 (0.0%)   | 0.86        | 1/3029 (0.0%)     |
| 47  | s     | 0.85         | 0/1142          | 1.24        | 4/1534 (0.3%)     |
| 48  | t     | 1.06         | 0/1745          | 1.24        | 1/2417 (0.0%)     |
| 49  | u     | 0.81         | 2/5475 (0.0%)   | 1.14        | 10/7432 (0.1%)    |
| 50  | v     | 0.86         | 0/2672          | 1.14        | 1/3647 (0.0%)     |
| 51  | w     | 0.38         | 0/1795          | 0.76        | 5/2798 (0.2%)     |
| 52  | x     | 0.88         | 0/2874          | 1.11        | 1/3925 (0.0%)     |
| 53  | y     | 0.78         | 0/5557          | 1.04        | 5/7503 (0.1%)     |
| All | All   | 0.73         | 6/114795 (0.0%) | 1.03        | 245/163973 (0.1%) |

All (6) bond length outliers are listed below:

| Mol | Chain | Res   | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-------|------|-------|-------|-------------|----------|
| 49  | u     | 14[A] | ARG  | C-O   | 7.72  | 1.33        | 1.24     |
| 49  | u     | 14[B] | ARG  | C-O   | 7.72  | 1.33        | 1.24     |
| 24  | P     | 140   | THR  | CA-C  | -5.49 | 1.45        | 1.52     |
| 24  | P     | 48    | SER  | CA-CB | -5.12 | 1.45        | 1.53     |
| 46  | r     | 231   | ALA  | N-CA  | 5.12  | 1.49        | 1.46     |
| 24  | P     | 103   | ASN  | CA-C  | -5.02 | 1.45        | 1.52     |

All (245) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 9   | A     | 1304 | U    | C2'-C3'-O3' | 14.11  | 134.87      | 113.70   |
| 24  | P     | 138  | ASP  | CA-CB-CG    | 14.02  | 126.62      | 112.60   |
| 24  | P     | 103  | ASN  | N-CA-C      | -12.11 | 98.51       | 113.28   |
| 47  | s     | 202  | PHE  | N-CA-C      | -12.06 | 98.09       | 112.92   |
| 9   | A     | 368  | U    | C2'-C3'-O3' | 11.08  | 126.12      | 109.50   |
| 9   | A     | 1867 | U    | C2'-C3'-O3' | 10.08  | 124.62      | 109.50   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 9   | A     | 1867 | U    | C4'-C3'-O3' | 9.93  | 124.29      | 109.40   |
| 9   | A     | 392  | A    | C2'-C3'-O3' | 9.88  | 128.51      | 113.70   |
| 1   | 1     | 396  | ASP  | CB-CA-C     | -9.72 | 96.87       | 112.03   |
| 9   | A     | 367  | U    | C2'-C3'-O3' | 9.67  | 128.21      | 113.70   |
| 1   | 1     | 677  | VAL  | N-CA-C      | -9.55 | 103.41      | 112.96   |
| 1   | 1     | 316  | THR  | CB-CA-C     | -9.54 | 94.92       | 111.05   |
| 9   | A     | 396  | U    | C2'-C3'-O3' | 8.99  | 127.18      | 113.70   |
| 9   | A     | 368  | U    | C4'-C3'-O3' | 8.92  | 122.78      | 109.40   |
| 41  | m     | 48   | HIS  | N-CA-C      | -8.80 | 103.05      | 113.88   |
| 10  | B     | 115  | PRO  | N-CA-C      | -8.67 | 101.94      | 113.65   |
| 53  | y     | 422  | GLU  | N-CA-C      | -8.64 | 97.09       | 109.96   |
| 10  | B     | 54   | THR  | N-CA-C      | -8.62 | 102.52      | 113.72   |
| 5   | 6     | 45   | ILE  | N-CA-C      | -8.60 | 104.83      | 111.62   |
| 9   | A     | 365  | C    | C2'-C3'-O3' | 8.55  | 126.53      | 113.70   |
| 1   | 1     | 648  | ILE  | N-CA-CB     | 8.51  | 125.27      | 111.23   |
| 39  | i     | 46   | TYR  | CB-CA-C     | 8.44  | 121.68      | 111.22   |
| 6   | 7     | 9    | A    | C2'-C3'-O3' | -8.39 | 101.11      | 113.70   |
| 9   | A     | 1302 | G    | C1'-C2'-O2' | 8.38  | 124.37      | 111.80   |
| 1   | 1     | 599  | LYS  | CB-CA-C     | -8.36 | 96.85       | 109.90   |
| 24  | P     | 137  | SER  | N-CA-C      | -8.28 | 102.12      | 112.72   |
| 1   | 1     | 396  | ASP  | N-CA-C      | -8.24 | 94.22       | 108.56   |
| 44  | p     | 53   | ASP  | N-CA-C      | -8.09 | 102.46      | 111.28   |
| 18  | J     | 77   | PRO  | N-CA-C      | -8.08 | 95.83       | 112.47   |
| 24  | P     | 121  | ARG  | N-CA-C      | -8.07 | 103.33      | 113.01   |
| 44  | p     | 107  | GLN  | N-CA-C      | -8.06 | 104.04      | 114.04   |
| 9   | A     | 393  | U    | C4'-C3'-O3' | 7.99  | 121.38      | 109.40   |
| 9   | A     | 366  | U    | C2'-C3'-O3' | 7.94  | 125.61      | 113.70   |
| 39  | i     | 12   | ARG  | N-CA-C      | -7.93 | 103.75      | 113.50   |
| 9   | A     | 1302 | G    | C3'-C2'-O2' | 7.84  | 126.37      | 114.60   |
| 49  | u     | 501  | THR  | N-CA-C      | -7.79 | 101.66      | 112.25   |
| 7   | 8     | 56   | GLU  | N-CA-C      | -7.72 | 102.06      | 113.40   |
| 21  | M     | 85   | VAL  | N-CA-C      | -7.64 | 100.64      | 108.96   |
| 1   | 1     | 427  | PRO  | N-CA-CB     | 7.61  | 111.24      | 103.25   |
| 9   | A     | 201  | C    | C2'-C3'-O3' | 7.56  | 125.04      | 113.70   |
| 24  | P     | 140  | THR  | N-CA-C      | -7.52 | 98.54       | 109.59   |
| 24  | P     | 138  | ASP  | N-CA-CB     | -7.45 | 99.24       | 110.35   |
| 1   | 1     | 327  | VAL  | CB-CA-C     | -7.42 | 105.40      | 111.71   |
| 44  | p     | 111  | HIS  | N-CA-C      | -7.38 | 104.15      | 113.01   |
| 31  | Z     | 58   | VAL  | N-CA-C      | -7.38 | 103.09      | 110.62   |
| 9   | A     | 373  | G    | C4'-C3'-O3' | 7.33  | 123.99      | 113.00   |
| 9   | A     | 1862 | G    | C4'-C3'-O3' | 7.31  | 120.37      | 109.40   |
| 9   | A     | 372  | U    | C2'-C3'-O3' | 7.29  | 124.63      | 113.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 49  | u     | 351  | LYS  | N-CA-C      | -7.18 | 104.25      | 113.16   |
| 1   | 1     | 427  | PRO  | N-CA-C      | -7.13 | 97.78       | 112.47   |
| 1   | 1     | 708  | PRO  | N-CA-C      | 7.07  | 117.26      | 110.47   |
| 52  | x     | 480  | ILE  | N-CA-C      | -7.05 | 105.67      | 112.29   |
| 45  | q     | 66   | ARG  | N-CA-C      | -7.03 | 103.82      | 112.88   |
| 9   | A     | 201  | C    | C4'-C3'-O3' | 6.92  | 123.38      | 113.00   |
| 13  | E     | 86   | PRO  | N-CA-C      | 6.89  | 123.33      | 113.47   |
| 1   | 1     | 699  | PHE  | N-CA-C      | -6.89 | 102.81      | 111.90   |
| 5   | 6     | 44   | GLN  | N-CA-C      | -6.88 | 103.24      | 112.94   |
| 1   | 1     | 316  | THR  | N-CA-C      | -6.86 | 96.43       | 108.23   |
| 1   | 1     | 618  | PRO  | N-CA-C      | -6.82 | 104.98      | 113.84   |
| 1   | 1     | 363  | GLU  | N-CA-C      | -6.78 | 104.87      | 113.01   |
| 45  | q     | 64   | LYS  | N-CA-C      | -6.77 | 103.90      | 111.28   |
| 11  | C     | 29   | PRO  | N-CA-C      | -6.75 | 100.64      | 111.03   |
| 41  | m     | 12   | MET  | N-CA-CB     | 6.69  | 121.06      | 110.49   |
| 14  | F     | 107  | LYS  | N-CA-C      | -6.68 | 104.00      | 111.28   |
| 40  | k     | 134  | SER  | N-CA-C      | -6.61 | 99.71       | 109.62   |
| 24  | P     | 117  | ARG  | N-CA-C      | -6.60 | 104.16      | 111.82   |
| 21  | M     | 71   | ILE  | N-CA-C      | 6.60  | 118.22      | 108.65   |
| 9   | A     | 392  | A    | C4'-C3'-O3' | 6.59  | 122.89      | 113.00   |
| 41  | m     | 34   | GLY  | CA-C-O      | -6.59 | 117.68      | 122.23   |
| 47  | s     | 270  | VAL  | N-CA-C      | -6.57 | 104.12      | 110.42   |
| 32  | a     | 4    | PRO  | N-CA-C      | -6.54 | 100.95      | 111.03   |
| 24  | P     | 147  | ARG  | N-CA-C      | -6.52 | 105.43      | 113.19   |
| 1   | 1     | 428  | ILE  | N-CA-C      | -6.47 | 102.96      | 111.05   |
| 29  | V     | 193  | LYS  | N-CA-C      | -6.47 | 104.23      | 111.28   |
| 9   | A     | 395  | G    | C4'-C3'-O3' | 6.42  | 122.63      | 113.00   |
| 44  | p     | 89   | GLN  | N-CA-C      | -6.41 | 105.75      | 112.93   |
| 51  | w     | 38   | C    | C2'-C3'-O3' | -6.41 | 104.09      | 113.70   |
| 43  | o     | 313  | GLU  | CB-CG-CD    | 6.38  | 123.44      | 112.60   |
| 9   | A     | 838  | G    | C5'-C4'-C3' | 6.37  | 124.76      | 115.20   |
| 9   | A     | 396  | U    | C4'-C3'-O3' | 6.37  | 122.55      | 113.00   |
| 51  | w     | 2    | G    | C2'-C3'-O3' | -6.36 | 104.17      | 113.70   |
| 9   | A     | 1308 | U    | C5'-C4'-C3' | 6.33  | 125.50      | 116.00   |
| 31  | Z     | 83   | SER  | N-CA-C      | -6.31 | 105.64      | 113.15   |
| 9   | A     | 1600 | G    | C4'-C3'-O3' | 6.29  | 118.84      | 109.40   |
| 21  | M     | 78   | ARG  | N-CA-C      | -6.28 | 103.71      | 111.75   |
| 9   | A     | 1307 | U    | N1-C1'-C2'  | 6.24  | 121.37      | 112.00   |
| 9   | A     | 370  | G    | C5'-C4'-C3' | 6.23  | 124.54      | 115.20   |
| 9   | A     | 996  | A    | C2'-C3'-O3' | -6.23 | 104.36      | 113.70   |
| 45  | q     | 84   | TYR  | N-CA-C      | -6.20 | 101.75      | 110.50   |
| 10  | B     | 99   | TYR  | CB-CA-C     | 6.20  | 121.62      | 109.72   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 1   | 1     | 557  | ASP  | CA-C-N      | -6.19 | 114.63      | 122.37   |
| 1   | 1     | 557  | ASP  | C-N-CA      | -6.19 | 114.63      | 122.37   |
| 24  | P     | 113  | GLN  | N-CA-C      | -6.19 | 105.22      | 112.89   |
| 31  | Z     | 211  | VAL  | N-CA-C      | -6.18 | 103.22      | 110.21   |
| 50  | v     | 312  | LEU  | N-CA-C      | -6.16 | 104.47      | 112.23   |
| 24  | P     | 81   | VAL  | N-CA-C      | -6.16 | 106.22      | 113.42   |
| 1   | 1     | 710  | THR  | CA-C-O      | -6.16 | 113.89      | 120.42   |
| 51  | w     | 35   | U    | C2'-C3'-O3' | 6.14  | 122.92      | 113.70   |
| 49  | u     | 277  | ASN  | N-CA-C      | -6.11 | 107.66      | 114.62   |
| 1   | 1     | 708  | PRO  | N-CA-CB     | -6.09 | 99.78       | 103.19   |
| 10  | B     | 48   | LYS  | N-CA-C      | -6.08 | 104.72      | 111.71   |
| 1   | 1     | 425  | HIS  | CA-C-N      | -6.03 | 115.86      | 123.15   |
| 1   | 1     | 425  | HIS  | C-N-CA      | -6.03 | 115.86      | 123.15   |
| 21  | M     | 73   | LEU  | CB-CA-C     | -6.02 | 100.80      | 110.79   |
| 41  | m     | 90   | GLY  | N-CA-C      | 6.02  | 120.02      | 113.58   |
| 41  | m     | 60   | MET  | N-CA-C      | -6.00 | 104.86      | 111.82   |
| 1   | 1     | 359  | LEU  | CA-C-N      | -5.97 | 112.53      | 122.21   |
| 1   | 1     | 359  | LEU  | C-N-CA      | -5.97 | 112.53      | 122.21   |
| 1   | 1     | 648  | ILE  | CA-C-N      | -5.96 | 112.46      | 122.29   |
| 1   | 1     | 648  | ILE  | C-N-CA      | -5.96 | 112.46      | 122.29   |
| 3   | 4     | 138  | PRO  | N-CA-C      | -5.93 | 101.88      | 111.19   |
| 29  | V     | 191  | LYS  | N-CA-C      | -5.93 | 104.81      | 111.28   |
| 6   | 7     | 28   | A    | C3'-C2'-O2' | -5.92 | 101.81      | 110.70   |
| 5   | 6     | 223  | LEU  | N-CA-C      | -5.89 | 104.29      | 112.30   |
| 21  | M     | 122  | PRO  | N-CA-C      | 5.88  | 120.72      | 111.38   |
| 5   | 6     | 149  | LYS  | N-CA-C      | -5.87 | 106.74      | 114.31   |
| 41  | m     | 11   | VAL  | CA-C-N      | -5.85 | 113.55      | 122.21   |
| 41  | m     | 11   | VAL  | C-N-CA      | -5.85 | 113.55      | 122.21   |
| 51  | w     | 73   | C    | C2'-C3'-O3' | -5.84 | 100.75      | 109.50   |
| 1   | 1     | 319  | PHE  | N-CA-C      | 5.82  | 118.70      | 109.50   |
| 29  | V     | 81   | ARG  | N-CA-C      | -5.81 | 106.23      | 113.38   |
| 1   | 1     | 571  | GLU  | N-CA-C      | -5.81 | 102.33      | 109.65   |
| 1   | 1     | 599  | LYS  | CA-C-O      | -5.80 | 114.31      | 120.92   |
| 21  | M     | 82   | ASP  | N-CA-C      | -5.79 | 105.05      | 111.71   |
| 1   | 1     | 513  | VAL  | N-CA-C      | -5.78 | 106.18      | 111.67   |
| 5   | 6     | 229  | VAL  | N-CA-C      | -5.77 | 106.59      | 111.56   |
| 1   | 1     | 307  | SER  | CA-C-N      | -5.76 | 115.28      | 122.48   |
| 1   | 1     | 307  | SER  | C-N-CA      | -5.76 | 115.28      | 122.48   |
| 49  | u     | 272  | MET  | N-CA-C      | -5.76 | 105.74      | 112.89   |
| 9   | A     | 1631 | U    | C5'-C4'-C3' | -5.74 | 107.39      | 116.00   |
| 7   | 8     | 53   | TYR  | N-CA-C      | -5.73 | 104.67      | 111.03   |
| 1   | 1     | 700  | CYS  | N-CA-C      | -5.72 | 104.96      | 111.14   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | N     | 7    | VAL  | N-CA-C      | -5.71 | 100.46      | 108.80   |
| 1   | 1     | 328  | SER  | N-CA-C      | 5.71  | 118.53      | 109.96   |
| 9   | A     | 372  | U    | C4'-C3'-O3' | 5.70  | 121.55      | 113.00   |
| 1   | 1     | 440  | ARG  | CA-C-N      | -5.67 | 114.89      | 122.72   |
| 1   | 1     | 440  | ARG  | C-N-CA      | -5.67 | 114.89      | 122.72   |
| 47  | s     | 200  | ARG  | N-CA-C      | -5.64 | 101.94      | 110.24   |
| 9   | A     | 374  | G    | C2'-C3'-O3' | 5.63  | 122.15      | 113.70   |
| 3   | 4     | 355  | VAL  | N-CA-C      | -5.61 | 106.98      | 111.81   |
| 1   | 1     | 309  | ILE  | N-CA-C      | -5.60 | 97.69       | 109.34   |
| 53  | y     | 669  | ARG  | N-CA-C      | -5.60 | 105.13      | 112.41   |
| 9   | A     | 393  | U    | N1-C1'-C2'  | 5.59  | 122.39      | 114.00   |
| 5   | 6     | 322  | TYR  | CA-C-O      | -5.58 | 115.31      | 121.28   |
| 8   | 9     | 6    | ARG  | N-CA-C      | -5.57 | 105.21      | 111.28   |
| 48  | t     | 168  | PRO  | N-CA-C      | 5.57  | 123.94      | 112.47   |
| 49  | u     | 286  | SER  | N-CA-C      | -5.56 | 105.80      | 112.59   |
| 10  | B     | 52   | GLU  | N-CA-C      | -5.55 | 106.28      | 113.16   |
| 3   | 4     | 167  | GLU  | N-CA-C      | 5.55  | 118.62      | 109.85   |
| 49  | u     | 271  | LEU  | N-CA-C      | -5.54 | 107.17      | 114.04   |
| 49  | u     | 562  | ARG  | N-CA-C      | -5.53 | 105.33      | 111.36   |
| 5   | 6     | 281  | THR  | N-CA-C      | -5.53 | 104.08      | 112.04   |
| 39  | i     | 50   | ILE  | N-CA-C      | -5.53 | 104.98      | 110.62   |
| 5   | 6     | 242  | THR  | N-CA-C      | -5.52 | 106.91      | 113.97   |
| 16  | H     | 16   | LYS  | N-CA-C      | -5.52 | 106.32      | 113.16   |
| 53  | y     | 744  | MET  | N-CA-C      | -5.51 | 106.23      | 113.12   |
| 5   | 6     | 48   | ALA  | N-CA-C      | -5.50 | 106.41      | 113.23   |
| 47  | s     | 251  | ASP  | N-CA-C      | -5.49 | 104.83      | 112.03   |
| 27  | S     | 204  | GLU  | CB-CA-C     | -5.49 | 102.44      | 110.95   |
| 9   | A     | 1301 | A    | C5'-C4'-C3' | 5.49  | 123.43      | 115.20   |
| 9   | A     | 1115 | U    | N1-C1'-C2'  | 5.47  | 120.21      | 112.00   |
| 15  | G     | 119  | SER  | N-CA-C      | -5.47 | 106.45      | 113.01   |
| 9   | A     | 1302 | G    | C5'-C4'-C3' | 5.47  | 123.40      | 115.20   |
| 1   | 1     | 309  | ILE  | CA-C-N      | -5.45 | 115.52      | 122.77   |
| 1   | 1     | 309  | ILE  | C-N-CA      | -5.45 | 115.52      | 122.77   |
| 9   | A     | 1453 | C    | N1-C1'-C2'  | 5.45  | 120.18      | 112.00   |
| 32  | a     | 74   | GLU  | N-CA-C      | -5.45 | 105.34      | 111.28   |
| 9   | A     | 200  | G    | C5'-C4'-C3' | 5.45  | 124.17      | 116.00   |
| 9   | A     | 366  | U    | C4'-C3'-O3' | 5.44  | 121.15      | 113.00   |
| 1   | 1     | 620  | GLY  | CA-C-O      | -5.43 | 117.89      | 122.29   |
| 29  | V     | 201  | LYS  | N-CA-C      | -5.41 | 105.38      | 111.28   |
| 5   | 6     | 227  | LYS  | N-CA-C      | -5.39 | 97.02       | 108.66   |
| 30  | Y     | 60   | LYS  | N-CA-C      | -5.39 | 105.41      | 111.28   |
| 1   | 1     | 582  | GLY  | N-CA-C      | 5.37  | 118.57      | 111.70   |

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| Mol | Chain | Res   | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-------|------|-------------|-------|-------------|----------|
| 24  | P     | 80    | ASP  | CA-C-N      | -5.36 | 115.47      | 121.85   |
| 24  | P     | 80    | ASP  | C-N-CA      | -5.36 | 115.47      | 121.85   |
| 44  | p     | 100   | ILE  | N-CA-C      | -5.36 | 105.73      | 113.07   |
| 41  | m     | 66    | GLU  | N-CA-C      | -5.36 | 105.44      | 111.28   |
| 1   | l     | 316   | THR  | O-C-N       | 5.35  | 129.74      | 122.57   |
| 9   | A     | 501   | C    | N1-C1'-C2'  | 5.35  | 120.02      | 112.00   |
| 9   | A     | 1     | U    | P-O3'-C3'   | 5.34  | 128.22      | 120.20   |
| 40  | k     | 105   | TYR  | CB-CA-C     | 5.34  | 119.93      | 110.85   |
| 9   | A     | 1359  | U    | C1'-C2'-O2' | -5.32 | 100.42      | 108.40   |
| 46  | r     | 80    | LYS  | N-CA-C      | -5.32 | 106.84      | 113.38   |
| 9   | A     | 197   | U    | C5'-C4'-C3' | 5.31  | 123.17      | 115.20   |
| 31  | Z     | 163   | PRO  | CB-CA-C     | -5.30 | 103.41      | 112.26   |
| 1   | l     | 327   | VAL  | O-C-N       | 5.30  | 125.88      | 121.85   |
| 37  | f     | 85    | ASN  | CB-CA-C     | -5.30 | 102.56      | 110.88   |
| 9   | A     | 367   | U    | C4'-C3'-O3' | 5.29  | 120.93      | 113.00   |
| 1   | l     | 649   | ALA  | N-CA-CB     | -5.28 | 101.71      | 111.53   |
| 31  | Z     | 211   | VAL  | CA-C-O      | -5.26 | 116.29      | 122.13   |
| 34  | c     | 273   | GLU  | CB-CG-CD    | 5.25  | 121.53      | 112.60   |
| 5   | 6     | 243   | ILE  | N-CA-C      | -5.24 | 106.78      | 112.80   |
| 9   | A     | 291   | G    | C2'-C3'-O3' | 5.24  | 121.55      | 113.70   |
| 49  | u     | 14[A] | ARG  | CA-C-O      | 5.22  | 125.95      | 120.42   |
| 49  | u     | 14[B] | ARG  | CA-C-O      | 5.22  | 125.95      | 120.42   |
| 45  | q     | 65    | LEU  | CA-C-N      | -5.21 | 114.47      | 122.60   |
| 45  | q     | 65    | LEU  | C-N-CA      | -5.21 | 114.47      | 122.60   |
| 9   | A     | 1825  | A    | C2'-C3'-O3' | -5.21 | 105.89      | 113.70   |
| 24  | P     | 101   | GLY  | CA-C-N      | -5.20 | 111.21      | 121.41   |
| 24  | P     | 101   | GLY  | C-N-CA      | -5.20 | 111.21      | 121.41   |
| 1   | l     | 648   | ILE  | CB-CA-C     | 5.19  | 119.81      | 111.29   |
| 53  | y     | 808   | SER  | N-CA-C      | -5.16 | 107.02      | 113.72   |
| 11  | C     | 235   | TRP  | N-CA-C      | -5.15 | 106.77      | 113.16   |
| 44  | p     | 87    | GLY  | CA-C-O      | -5.15 | 118.45      | 122.52   |
| 21  | M     | 81    | ARG  | N-CA-C      | -5.14 | 106.86      | 113.02   |
| 1   | l     | 396   | ASP  | CA-C-O      | -5.13 | 116.47      | 122.37   |
| 1   | l     | 485   | GLU  | N-CA-C      | 5.13  | 117.67      | 110.23   |
| 9   | A     | 1642  | U    | C3'-C2'-O2' | 5.13  | 118.40      | 110.70   |
| 5   | 6     | 15    | ALA  | N-CA-C      | 5.13  | 118.70      | 111.52   |
| 24  | P     | 139   | SER  | CA-C-N      | -5.12 | 113.86      | 121.24   |
| 24  | P     | 139   | SER  | C-N-CA      | -5.12 | 113.86      | 121.24   |
| 24  | P     | 145   | GLY  | CA-C-O      | -5.12 | 117.86      | 122.57   |
| 51  | w     | 40    | C    | C1'-C2'-O2' | 5.12  | 116.09      | 108.40   |
| 1   | l     | 384   | CYS  | N-CA-C      | -5.12 | 106.62      | 112.92   |
| 9   | A     | 688   | U    | C2'-C3'-O3' | 5.11  | 117.17      | 109.50   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 30  | Y     | 74   | GLY  | CA-C-O      | -5.11 | 118.15      | 122.29   |
| 32  | a     | 62   | PHE  | CA-C-O      | -5.11 | 115.99      | 121.56   |
| 7   | 8     | 274  | LYS  | N-CA-C      | -5.11 | 106.31      | 112.54   |
| 44  | p     | 63   | PHE  | N-CA-C      | -5.11 | 105.61      | 111.07   |
| 49  | u     | 507  | ILE  | N-CA-C      | -5.10 | 101.72      | 109.78   |
| 9   | A     | 839  | C    | C2'-C3'-O3' | -5.10 | 101.86      | 109.50   |
| 5   | 6     | 49   | CYS  | N-CA-C      | -5.09 | 107.02      | 113.18   |
| 12  | D     | 138  | ARG  | CB-CA-C     | 5.08  | 119.11      | 111.89   |
| 1   | 1     | 395  | MET  | N-CA-C      | 5.08  | 118.23      | 110.20   |
| 11  | C     | 27   | PHE  | CB-CA-C     | 5.07  | 118.51      | 110.19   |
| 22  | N     | 102  | ARG  | CA-CB-CG    | -5.07 | 103.97      | 114.10   |
| 24  | P     | 136  | PRO  | CB-CA-C     | -5.06 | 103.20      | 111.56   |
| 53  | y     | 271  | GLU  | N-CA-C      | -5.06 | 105.84      | 111.36   |
| 29  | V     | 137  | GLN  | CA-C-O      | -5.06 | 115.34      | 120.71   |
| 9   | A     | 203  | G    | C5'-C4'-C3' | 5.06  | 122.79      | 115.20   |
| 9   | A     | 395  | G    | C2'-C3'-O3' | 5.05  | 121.27      | 113.70   |
| 23  | O     | 116  | LYS  | CA-C-O      | -5.05 | 115.51      | 121.16   |
| 25  | Q     | 15   | ARG  | CG-CD-NE    | 5.04  | 123.10      | 112.00   |
| 1   | 1     | 317  | SER  | N-CA-C      | 5.04  | 117.71      | 109.59   |
| 31  | Z     | 56   | GLN  | CB-CG-CD    | 5.04  | 121.17      | 112.60   |
| 1   | 1     | 598  | GLY  | CA-C-O      | -5.03 | 114.12      | 119.55   |
| 29  | V     | 194  | ASP  | CA-C-O      | -5.02 | 115.23      | 120.55   |
| 45  | q     | 48   | GLU  | N-CA-C      | -5.02 | 103.90      | 110.53   |
| 9   | A     | 1310 | U    | C2'-C3'-O3' | -5.02 | 106.17      | 113.70   |
| 1   | 1     | 679  | ASN  | N-CA-C      | -5.02 | 100.21      | 108.49   |
| 7   | 8     | 205  | ILE  | N-CA-C      | -5.02 | 106.56      | 111.88   |
| 40  | k     | 122  | PRO  | N-CA-C      | -5.01 | 102.04      | 112.36   |
| 1   | 1     | 447  | SER  | CA-C-N      | -5.00 | 116.99      | 123.19   |
| 1   | 1     | 447  | SER  | C-N-CA      | -5.00 | 116.99      | 123.19   |

There are no chirality outliers.

There are no planarity outliers.

## 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   | 1     | 2445  | 0        | 1563     | 42      | 0            |
| 2   | 3     | 1057  | 0        | 475      | 12      | 0            |
| 3   | 4     | 1272  | 0        | 564      | 22      | 0            |
| 4   | 5     | 1581  | 0        | 689      | 9       | 0            |
| 5   | 6     | 1917  | 0        | 1096     | 36      | 0            |
| 6   | 7     | 240   | 0        | 121      | 0       | 0            |
| 7   | 8     | 1571  | 0        | 683      | 14      | 0            |
| 8   | 9     | 230   | 0        | 276      | 7       | 0            |
| 9   | A     | 36668 | 0        | 18551    | 639     | 0            |
| 10  | B     | 1166  | 0        | 1233     | 36      | 0            |
| 11  | C     | 2035  | 0        | 2138     | 72      | 0            |
| 12  | D     | 1477  | 0        | 1589     | 36      | 0            |
| 13  | E     | 1087  | 0        | 1154     | 18      | 0            |
| 14  | F     | 330   | 0        | 373      | 11      | 0            |
| 15  | G     | 1430  | 0        | 1520     | 50      | 0            |
| 16  | H     | 631   | 0        | 657      | 31      | 0            |
| 17  | I     | 1208  | 0        | 1294     | 34      | 0            |
| 18  | J     | 1034  | 0        | 1080     | 25      | 0            |
| 19  | K     | 617   | 0        | 622      | 20      | 0            |
| 20  | L     | 1707  | 0        | 1794     | 55      | 0            |
| 21  | M     | 1064  | 0        | 1118     | 59      | 0            |
| 22  | N     | 1633  | 0        | 1640     | 51      | 0            |
| 23  | O     | 1715  | 0        | 1785     | 52      | 0            |
| 24  | P     | 997   | 0        | 1021     | 62      | 0            |
| 25  | Q     | 792   | 0        | 843      | 36      | 0            |
| 26  | R     | 1627  | 0        | 1706     | 44      | 0            |
| 27  | S     | 1862  | 0        | 2018     | 55      | 0            |
| 28  | T     | 1015  | 0        | 1086     | 37      | 0            |
| 29  | V     | 1461  | 0        | 1511     | 54      | 0            |
| 30  | Y     | 1124  | 0        | 1193     | 53      | 0            |
| 31  | Z     | 1765  | 0        | 1865     | 47      | 0            |
| 32  | a     | 834   | 0        | 861      | 28      | 0            |
| 33  | b     | 913   | 0        | 952      | 35      | 0            |
| 34  | c     | 2436  | 0        | 2393     | 53      | 0            |
| 35  | d     | 1105  | 0        | 1138     | 31      | 0            |
| 36  | e     | 523   | 0        | 573      | 19      | 0            |
| 37  | f     | 1176  | 0        | 1233     | 44      | 0            |
| 38  | h     | 817   | 0        | 882      | 12      | 0            |
| 39  | i     | 419   | 0        | 415      | 26      | 0            |
| 40  | k     | 435   | 0        | 434      | 30      | 0            |
| 41  | m     | 950   | 0        | 987      | 37      | 0            |
| 42  | n     | 498   | 0        | 525      | 23      | 0            |
| 43  | o     | 616   | 0        | 600      | 15      | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 44  | p     | 691    | 0        | 706      | 36      | 0            |
| 45  | q     | 714    | 0        | 735      | 41      | 0            |
| 46  | r     | 2215   | 0        | 2266     | 43      | 0            |
| 47  | s     | 1123   | 0        | 1157     | 35      | 0            |
| 48  | t     | 1750   | 0        | 806      | 14      | 0            |
| 49  | u     | 5383   | 0        | 5085     | 112     | 0            |
| 50  | v     | 2635   | 0        | 2207     | 54      | 0            |
| 51  | w     | 1604   | 0        | 816      | 23      | 0            |
| 52  | x     | 2831   | 0        | 2199     | 50      | 0            |
| 53  | y     | 5470   | 0        | 5329     | 104     | 0            |
| 54  | Q     | 1      | 0        | 0        | 0       | 0            |
| 54  | k     | 1      | 0        | 0        | 0       | 0            |
| 55  | d     | 1      | 0        | 0        | 0       | 0            |
| 55  | f     | 1      | 0        | 0        | 0       | 0            |
| All | All   | 109900 | 0        | 85557    | 1938    | 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 11.

All (1938) 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) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:B:35:ARG:HH21  | 10:B:51:ILE:HA    | 1.09                     | 1.16              |
| 41:m:100:PRO:HB2  | 41:m:103:VAL:HB   | 1.38                     | 1.05              |
| 10:B:35:ARG:NH2   | 10:B:51:ILE:HG23  | 1.71                     | 1.03              |
| 10:B:35:ARG:HH22  | 10:B:51:ILE:HG23  | 1.23                     | 0.96              |
| 24:P:66:ARG:HH12  | 46:r:53:ARG:HB2   | 1.30                     | 0.93              |
| 31:Z:89:GLU:HB3   | 43:o:309:ILE:HB   | 1.49                     | 0.93              |
| 29:V:102:LEU:HD11 | 36:e:100:VAL:HG21 | 1.53                     | 0.91              |
| 9:A:307:G:C6      | 26:R:44:HIS:CD2   | 2.60                     | 0.90              |
| 21:M:79:GLU:HA    | 21:M:82:ASP:HB2   | 1.52                     | 0.89              |
| 9:A:570:C:H4'     | 28:T:36:PRO:HG3   | 1.55                     | 0.88              |
| 11:C:161:GLN:HB3  | 11:C:170:THR:HB   | 1.56                     | 0.87              |
| 10:B:35:ARG:NH2   | 10:B:51:ILE:HA    | 1.89                     | 0.86              |
| 9:A:687:C:H5''    | 15:G:123:THR:HG21 | 1.56                     | 0.86              |
| 10:B:120:VAL:HG12 | 10:B:145:VAL:HG11 | 1.57                     | 0.86              |
| 10:B:5:GLN:NE2    | 10:B:7:GLU:O      | 2.10                     | 0.85              |
| 46:r:183:ARG:NH1  | 51:w:53:A:N3      | 2.25                     | 0.85              |
| 50:v:347:ILE:HG23 | 53:y:826:ILE:HD12 | 1.59                     | 0.85              |
| 9:A:448:A:H5''    | 26:R:25:ARG:HA    | 1.56                     | 0.85              |
| 9:A:688:U:C5      | 15:G:122:LEU:HB2  | 2.13                     | 0.84              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:A:1033:G:H1     | 9:A:1080:A:HO2'   | 1.26                     | 0.83              |
| 32:a:26:ASP:HB3   | 32:a:29:MET:HB2   | 1.60                     | 0.83              |
| 9:A:1016:U:N3     | 17:I:17:PRO:HG3   | 1.94                     | 0.82              |
| 9:A:1114:U:O2     | 23:O:203:SER:HB3  | 1.78                     | 0.82              |
| 35:d:35:ASP:HB2   | 37:f:46:ARG:HG2   | 1.61                     | 0.82              |
| 29:V:140:ASP:HB2  | 42:n:46:VAL:HG12  | 1.62                     | 0.81              |
| 47:s:188:ARG:HH11 | 47:s:194:MET:HA   | 1.47                     | 0.81              |
| 9:A:377:G:H5'     | 26:R:98:LYS:HB3   | 1.63                     | 0.80              |
| 1:1:330:GLU:CB    | 1:1:364:LYS:HA    | 2.10                     | 0.80              |
| 9:A:925:G:H1      | 9:A:1017:U:H3     | 1.25                     | 0.80              |
| 9:A:802:A:H62     | 15:G:106:ARG:NH1  | 1.79                     | 0.80              |
| 9:A:352:U:H5''    | 10:B:139:ARG:HG2  | 1.64                     | 0.80              |
| 9:A:688:U:C6      | 15:G:122:LEU:HB2  | 2.17                     | 0.80              |
| 9:A:1711:U:H5''   | 45:q:58:LEU:HD11  | 1.63                     | 0.80              |
| 9:A:1016:U:H3     | 17:I:17:PRO:HG3   | 1.47                     | 0.79              |
| 15:G:69:LEU:HD13  | 15:G:96:ALA:HB2   | 1.63                     | 0.79              |
| 9:A:1679:A:H2'    | 29:V:60:ARG:HD2   | 1.65                     | 0.78              |
| 9:A:841:G:OP2     | 28:T:14:THR:N     | 2.15                     | 0.78              |
| 9:A:1154:U:O2'    | 20:L:194:ARG:HD2  | 1.84                     | 0.78              |
| 11:C:188:ASN:HB3  | 11:C:191:ARG:HD3  | 1.65                     | 0.78              |
| 21:M:109:LEU:HD11 | 22:N:52:LYS:HB2   | 1.66                     | 0.78              |
| 31:Z:227:LYS:HD2  | 34:c:184:LEU:HD23 | 1.64                     | 0.78              |
| 9:A:1398:G:O2'    | 34:c:88:ARG:NH2   | 2.16                     | 0.77              |
| 12:D:54:ARG:HH12  | 20:L:202:THR:HG22 | 1.47                     | 0.76              |
| 34:c:87:LEU:HB2   | 34:c:101:PHE:HB2  | 1.66                     | 0.76              |
| 41:m:14:VAL:HG21  | 41:m:126:GLU:HG3  | 1.67                     | 0.76              |
| 44:p:47:VAL:HB    | 44:p:83:ILE:HB    | 1.68                     | 0.76              |
| 9:A:77:A:H2       | 27:S:175:LYS:HG3  | 1.51                     | 0.76              |
| 9:A:641:A:OP1     | 12:D:40:LYS:NZ    | 2.18                     | 0.76              |
| 40:k:133:ALA:HB3  | 40:k:140:TYR:HB3  | 1.68                     | 0.76              |
| 52:x:359:ARG:H    | 52:x:375:CYS:HB2  | 1.51                     | 0.76              |
| 9:A:984:C:O2      | 24:P:138:ASP:HB2  | 1.85                     | 0.76              |
| 41:m:79:VAL:HG21  | 41:m:85:LEU:HB2   | 1.68                     | 0.75              |
| 40:k:139:HIS:HB3  | 40:k:148:TYR:HB3  | 1.68                     | 0.75              |
| 9:A:1569:A:H5'    | 35:d:41:LYS:HD3   | 1.68                     | 0.75              |
| 9:A:1156:U:OP1    | 18:J:71:LYS:NZ    | 2.19                     | 0.75              |
| 9:A:1153:C:OP2    | 18:J:71:LYS:HE3   | 1.86                     | 0.75              |
| 27:S:135:PRO:HB2  | 27:S:141:ILE:HG12 | 1.69                     | 0.74              |
| 9:A:1358:U:OP2    | 20:L:123:ARG:NH1  | 2.19                     | 0.74              |
| 9:A:1566:G:OP2    | 35:d:102:ARG:NH1  | 2.20                     | 0.74              |
| 46:r:196:GLU:HG3  | 46:r:234:ARG:HA   | 1.69                     | 0.74              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:M:114:LEU:HD22 | 22:N:16:LEU:HD21  | 1.69                     | 0.74              |
| 9:A:4:C:H1'       | 12:D:18:ARG:HH12  | 1.51                     | 0.74              |
| 9:A:687:C:H5''    | 15:G:123:THR:CG2  | 2.16                     | 0.74              |
| 9:A:1016:U:H5''   | 17:I:14:SER:HB2   | 1.68                     | 0.74              |
| 9:A:1077:A:O2'    | 53:y:51:SER:HB3   | 1.88                     | 0.73              |
| 9:A:1541:G:N3     | 35:d:12:GLN:NE2   | 2.35                     | 0.73              |
| 9:A:1522:A:OP1    | 37:f:144:ARG:NH2  | 2.20                     | 0.73              |
| 11:C:41:CYS:HB2   | 11:C:83:PRO:HB2   | 1.71                     | 0.73              |
| 1:1:565:ILE:HD11  | 1:1:579:VAL:HB    | 1.69                     | 0.73              |
| 9:A:955:A:H4'     | 24:P:60:MET:HE3   | 1.69                     | 0.73              |
| 9:A:1004:U:P      | 23:O:165:ARG:HH21 | 2.11                     | 0.73              |
| 40:k:141:CYS:HB2  | 40:k:147:THR:HA   | 1.69                     | 0.73              |
| 5:6:308:VAL:HA    | 5:6:311:PHE:HB3   | 1.70                     | 0.73              |
| 9:A:161:U:H5'     | 28:T:116:LYS:HB3  | 1.69                     | 0.73              |
| 10:B:134:LEU:HB2  | 10:B:138:VAL:HB   | 1.70                     | 0.73              |
| 9:A:1416:C:H4'    | 35:d:132:ASP:HB3  | 1.71                     | 0.72              |
| 9:A:1661:A:C8     | 39:i:14:PHE:HB2   | 2.24                     | 0.72              |
| 5:6:357:TRP:CZ3   | 7:8:352:ASN:HA    | 2.25                     | 0.72              |
| 24:P:28:PHE:HZ    | 25:Q:58:VAL:HG21  | 1.53                     | 0.72              |
| 40:k:141:CYS:HB3  | 40:k:144:CYS:HB2  | 1.69                     | 0.72              |
| 9:A:928:G:H1      | 9:A:1013:U:H3     | 1.35                     | 0.72              |
| 10:B:35:ARG:HH21  | 10:B:51:ILE:CA    | 1.97                     | 0.72              |
| 9:A:551:U:H5'     | 14:F:117:VAL:HG11 | 1.72                     | 0.72              |
| 9:A:1825:A:H2'    | 45:q:44:ASN:HB3   | 1.70                     | 0.72              |
| 9:A:1399:C:H5''   | 34:c:100:ARG:CZ   | 2.20                     | 0.72              |
| 9:A:957:A:H5''    | 24:P:57:THR:HG21  | 1.72                     | 0.71              |
| 25:Q:89:ARG:HA    | 25:Q:92:ARG:HD2   | 1.70                     | 0.71              |
| 29:V:48:TYR:HD2   | 30:Y:53:GLU:HG2   | 1.55                     | 0.71              |
| 33:b:108:LYS:HZ2  | 37:f:116:LYS:HG2  | 1.54                     | 0.71              |
| 29:V:142:SER:HB2  | 42:n:50:VAL:HG22  | 1.71                     | 0.71              |
| 9:A:688:U:OP1     | 15:G:122:LEU:N    | 2.24                     | 0.71              |
| 10:B:35:ARG:NH2   | 10:B:51:ILE:CG2   | 2.52                     | 0.71              |
| 9:A:1091:C:HO2'   | 18:J:2:VAL:N      | 1.87                     | 0.71              |
| 46:r:194:ASP:HA   | 46:r:236:VAL:HA   | 1.72                     | 0.71              |
| 9:A:574:A:H4'     | 28:T:89:HIS:CG    | 2.26                     | 0.71              |
| 9:A:1093:A:H5''   | 18:J:28:ARG:HH22  | 1.56                     | 0.71              |
| 9:A:1606:G:H1     | 9:A:1632:G:HO2'   | 1.39                     | 0.71              |
| 21:M:111:PHE:CZ   | 22:N:15:VAL:HG21  | 2.26                     | 0.71              |
| 9:A:1609:C:H5''   | 37:f:131:VAL:HG22 | 1.70                     | 0.71              |
| 9:A:453:C:O2'     | 27:S:92:ARG:O     | 2.08                     | 0.70              |
| 9:A:1373:C:OP1    | 21:M:7:LYS:N      | 2.23                     | 0.70              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 41:m:51:VAL:HG13  | 41:m:109:VAL:HG13 | 1.73                     | 0.70              |
| 29:V:122:ARG:HD2  | 42:n:57:THR:HG21  | 1.73                     | 0.70              |
| 41:m:42:LEU:HD11  | 41:m:74:ILE:HD13  | 1.74                     | 0.70              |
| 53:y:831:LEU:HG   | 53:y:844:MET:HB2  | 1.72                     | 0.70              |
| 9:A:919:A:OP2     | 17:I:64:ARG:NH2   | 2.24                     | 0.70              |
| 9:A:1350:U:O2     | 22:N:110:ASN:ND2  | 2.25                     | 0.70              |
| 9:A:860:G:H21     | 18:J:107:SER:HG   | 1.39                     | 0.70              |
| 53:y:421:GLY:HA2  | 53:y:440:VAL:HA   | 1.74                     | 0.70              |
| 9:A:802:A:H62     | 15:G:106:ARG:HH11 | 1.38                     | 0.69              |
| 16:H:24:LEU:HD11  | 18:J:53:ILE:HG12  | 1.74                     | 0.69              |
| 9:A:142:C:OP2     | 27:S:188:LYS:NZ   | 2.25                     | 0.69              |
| 11:C:11:ARG:HH11  | 11:C:21:ASP:H     | 1.38                     | 0.69              |
| 27:S:142:ARG:HA   | 27:S:147:LEU:HB2  | 1.74                     | 0.69              |
| 40:k:138:ARG:HH21 | 40:k:140:TYR:HB2  | 1.57                     | 0.69              |
| 1:l:548:ARG:HB2   | 1:l:555:PRO:HD2   | 1.74                     | 0.69              |
| 9:A:376:A:N3      | 26:R:86:SER:OG    | 2.24                     | 0.69              |
| 9:A:676:C:H5''    | 17:I:5:HIS:CD2    | 2.28                     | 0.69              |
| 9:A:1334:G:O3'    | 31:Z:183:GLY:HA3  | 1.93                     | 0.69              |
| 19:K:41:LYS:HA    | 22:N:5:LEU:HD12   | 1.74                     | 0.69              |
| 9:A:1252:C:OP1    | 38:h:75:LYS:HE2   | 1.93                     | 0.69              |
| 16:H:78:SER:HA    | 52:x:79:SER:O     | 1.93                     | 0.69              |
| 21:M:77:GLU:HA    | 21:M:80:ARG:HB3   | 1.75                     | 0.69              |
| 44:p:35:ILE:HD11  | 44:p:90:ARG:HB2   | 1.74                     | 0.69              |
| 52:x:82:LEU:HD11  | 53:y:665:VAL:HG21 | 1.73                     | 0.69              |
| 23:O:67:PHE:CE1   | 24:P:48:SER:HB3   | 2.27                     | 0.69              |
| 4:5:291:ILE:CB    | 4:5:443:GLN:HA    | 2.22                     | 0.68              |
| 9:A:1513:C:OP1    | 39:i:9:SER:HB2    | 1.93                     | 0.68              |
| 9:A:643:A:OP1     | 12:D:38:ARG:NH1   | 2.26                     | 0.68              |
| 46:r:231:ALA:HB3  | 46:r:234:ARG:HB3  | 1.75                     | 0.68              |
| 49:u:405:GLU:HA   | 49:u:408:THR:HG22 | 1.76                     | 0.68              |
| 9:A:1248:U:H2'    | 9:A:1249:C:C6     | 2.28                     | 0.68              |
| 9:A:932:G:OP1     | 23:O:158:HIS:N    | 2.24                     | 0.68              |
| 31:Z:42:THR:HG22  | 31:Z:45:ARG:H     | 1.58                     | 0.68              |
| 53:y:64:ILE:HG12  | 53:y:109:ILE:HD11 | 1.74                     | 0.68              |
| 9:A:987:A:OP1     | 25:Q:32:LYS:NZ    | 2.26                     | 0.68              |
| 13:E:88:ASP:OD1   | 14:F:84:GLY:HA2   | 1.94                     | 0.68              |
| 31:Z:20:GLU:HB2   | 32:a:64:TRP:CE3   | 2.29                     | 0.68              |
| 24:P:57:THR:HB    | 24:P:60:MET:HG3   | 1.76                     | 0.67              |
| 9:A:751:G:H22     | 9:A:789:G:H5''    | 1.58                     | 0.67              |
| 37:f:34:LYS:HB3   | 37:f:100:ALA:HA   | 1.76                     | 0.67              |
| 29:V:49:LEU:HD13  | 30:Y:47:LEU:HA    | 1.76                     | 0.67              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 31:Z:16:ILE:HD11  | 39:i:36:LEU:HD23  | 1.76                     | 0.67              |
| 50:v:290:ASP:HB3  | 50:v:293:THR:HB   | 1.74                     | 0.67              |
| 49:u:296:LEU:HB3  | 49:u:322:VAL:HG23 | 1.76                     | 0.67              |
| 32:a:20:VAL:HG12  | 32:a:70:TYR:HA    | 1.75                     | 0.67              |
| 9:A:1648:G:H5'    | 30:Y:125:ARG:HB3  | 1.76                     | 0.67              |
| 9:A:687:C:O2'     | 15:G:116:ARG:NH2  | 2.27                     | 0.67              |
| 25:Q:11:ALA:HB3   | 25:Q:33:ASP:HB2   | 1.76                     | 0.67              |
| 5:6:357:TRP:HZ3   | 7:8:352:ASN:HA    | 1.57                     | 0.66              |
| 47:s:296:ARG:HH12 | 51:w:69:G:H3'     | 1.58                     | 0.66              |
| 47:s:296:ARG:NH2  | 51:w:69:G:OP2     | 2.28                     | 0.66              |
| 31:Z:59:LEU:HA    | 31:Z:66:ILE:HG12  | 1.77                     | 0.66              |
| 34:c:174:VAL:HB   | 34:c:188:HIS:HB2  | 1.76                     | 0.66              |
| 9:A:837:A:H5'     | 9:A:839:C:OP1     | 1.95                     | 0.66              |
| 9:A:922:A:OP2     | 18:J:28:ARG:NH1   | 2.28                     | 0.66              |
| 9:A:925:G:H5'     | 17:I:121:ARG:HH12 | 1.58                     | 0.66              |
| 1:1:335:TRP:HA    | 1:1:367:GLN:CB    | 2.25                     | 0.66              |
| 9:A:688:U:H3'     | 15:G:103:LYS:HD2  | 1.77                     | 0.66              |
| 9:A:1556:A:N1     | 39:i:13:LYS:HA    | 2.10                     | 0.66              |
| 9:A:1348:G:OP1    | 20:L:145:LYS:NZ   | 2.28                     | 0.66              |
| 9:A:1648:G:C5'    | 30:Y:125:ARG:HB3  | 2.26                     | 0.66              |
| 31:Z:16:ILE:HD11  | 39:i:36:LEU:HA    | 1.76                     | 0.66              |
| 41:m:91:LEU:HD13  | 41:m:104:VAL:HB   | 1.78                     | 0.66              |
| 43:o:269:TYR:HB3  | 43:o:284:PHE:HB2  | 1.77                     | 0.66              |
| 1:1:360:TRP:CB    | 1:1:367:GLN:HA    | 2.25                     | 0.66              |
| 9:A:801:U:H5      | 15:G:106:ARG:HH22 | 1.42                     | 0.66              |
| 9:A:1047:C:H5'    | 24:P:143:LYS:HB2  | 1.78                     | 0.66              |
| 9:A:1377:U:C4     | 22:N:102:ARG:CZ   | 2.78                     | 0.66              |
| 9:A:1379:A:O2'    | 22:N:105:PRO:HD2  | 1.94                     | 0.66              |
| 9:A:1417:C:O2'    | 35:d:3:GLY:HA2    | 1.96                     | 0.65              |
| 9:A:77:A:H1'      | 27:S:176:ILE:HG13 | 1.78                     | 0.65              |
| 9:A:1300:U:O2     | 33:b:51:ARG:HD3   | 1.96                     | 0.65              |
| 31:Z:223:ILE:HG23 | 34:c:189:ILE:HD12 | 1.79                     | 0.65              |
| 45:q:41:MET:HG2   | 45:q:47:LEU:HD13  | 1.77                     | 0.65              |
| 52:x:378:ASP:HB2  | 52:x:393:ILE:H    | 1.61                     | 0.65              |
| 40:k:138:ARG:HG3  | 40:k:149:CYS:HA   | 1.79                     | 0.65              |
| 8:9:1:MET:HE1     | 8:9:9:ARG:HD3     | 1.79                     | 0.65              |
| 9:A:528:A:N1      | 9:A:557:U:O2'     | 2.30                     | 0.65              |
| 9:A:1587:G:C5     | 35:d:67:ARG:HD3   | 2.32                     | 0.65              |
| 27:S:32:MET:HB2   | 27:S:100:CYS:HB2  | 1.78                     | 0.65              |
| 9:A:1378:A:N6     | 22:N:136:GLU:OE2  | 2.29                     | 0.64              |
| 12:D:33:GLY:HA3   | 14:F:112:TYR:CD1  | 2.32                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 48:t:418:SER:H    | 48:t:427:ILE:HA   | 1.61                     | 0.64              |
| 9:A:887:U:H2'     | 9:A:888:U:H2'     | 1.78                     | 0.64              |
| 30:Y:27:ARG:HA    | 30:Y:66:VAL:HG12  | 1.80                     | 0.64              |
| 9:A:860:G:N2      | 18:J:107:SER:HG   | 1.95                     | 0.64              |
| 40:k:133:ALA:HB3  | 40:k:140:TYR:CG   | 2.33                     | 0.64              |
| 49:u:329:ILE:HB   | 49:u:367:ARG:HH11 | 1.62                     | 0.64              |
| 2:3:152:HIS:O     | 4:5:506:ILE:O     | 2.15                     | 0.64              |
| 30:Y:132:PHE:HB2  | 38:h:77:TRP:CD1   | 2.32                     | 0.64              |
| 9:A:1683:C:C2     | 42:n:24:GLN:HG3   | 2.33                     | 0.64              |
| 3:4:107:GLU:O     | 49:u:571:ARG:HB2  | 1.98                     | 0.64              |
| 9:A:957:A:C5'     | 24:P:57:THR:HG21  | 2.28                     | 0.64              |
| 41:m:81:ASP:HB3   | 41:m:84:LYS:HB2   | 1.79                     | 0.64              |
| 42:n:20:ARG:HA    | 42:n:28:THR:HA    | 1.80                     | 0.64              |
| 23:O:128:LYS:HE3  | 53:y:308:VAL:HA   | 1.81                     | 0.63              |
| 9:A:1745:A:H1'    | 27:S:66:GLY:HA2   | 1.80                     | 0.63              |
| 9:A:835:C:H5''    | 9:A:836:G:H5'     | 1.79                     | 0.63              |
| 9:A:1047:C:O3'    | 24:P:143:LYS:HA   | 1.98                     | 0.63              |
| 11:C:54:TYR:O     | 28:T:15:ASN:ND2   | 2.31                     | 0.63              |
| 52:x:452:VAL:HG22 | 52:x:465:ILE:HG22 | 1.81                     | 0.63              |
| 34:c:5:MET:HE2    | 34:c:312:VAL:HB   | 1.80                     | 0.63              |
| 11:C:36:HIS:CD2   | 11:C:85:GLY:HA3   | 2.33                     | 0.63              |
| 21:M:78:ARG:HH21  | 22:N:89:LYS:NZ    | 1.96                     | 0.63              |
| 50:v:349:GLN:HB2  | 53:y:833:ALA:HB1  | 1.81                     | 0.63              |
| 52:x:391:ILE:HG22 | 52:x:446:TYR:HB2  | 1.79                     | 0.63              |
| 9:A:1024:A:OP2    | 17:I:124:ARG:NH1  | 2.25                     | 0.63              |
| 9:A:72:C:O2'      | 9:A:74:G:N2       | 2.31                     | 0.63              |
| 9:A:1464:C:H4'    | 21:M:60:ARG:HH21  | 1.64                     | 0.63              |
| 11:C:228:ILE:HB   | 11:C:236:ILE:HD11 | 1.80                     | 0.63              |
| 18:J:95:PRO:HB2   | 20:L:182:CYS:SG   | 2.38                     | 0.63              |
| 24:P:150:ARG:H    | 24:P:150:ARG:HE   | 1.46                     | 0.63              |
| 53:y:68:ARG:HH12  | 53:y:109:ILE:HA   | 1.61                     | 0.63              |
| 45:q:28:PHE:HD1   | 45:q:29:LYS:HG2   | 1.64                     | 0.63              |
| 9:A:72:C:H42      | 27:S:170:ARG:HG3  | 1.64                     | 0.63              |
| 9:A:1543:U:OP1    | 35:d:62:ARG:NH2   | 2.30                     | 0.63              |
| 24:P:57:THR:HG22  | 24:P:59:GLY:H     | 1.63                     | 0.63              |
| 9:A:921:G:H5'     | 16:H:21:LYS:NZ    | 2.14                     | 0.62              |
| 10:B:109:MET:CE   | 10:B:140:PHE:CE1  | 2.82                     | 0.62              |
| 9:A:67:C:C5       | 27:S:162:LEU:HB3  | 2.33                     | 0.62              |
| 9:A:752:G:N2      | 9:A:793:G:O2'     | 2.32                     | 0.62              |
| 43:o:304:GLY:HA2  | 43:o:309:ILE:HA   | 1.79                     | 0.62              |
| 10:B:35:ARG:HH22  | 10:B:51:ILE:CG2   | 2.07                     | 0.62              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 19:K:9:VAL:HG21   | 20:L:177:PRO:HD3  | 1.80                     | 0.62              |
| 52:x:289:LEU:HD23 | 52:x:316:ALA:HB1  | 1.81                     | 0.62              |
| 9:A:1631:U:H4'    | 37:f:34:LYS:HE3   | 1.81                     | 0.62              |
| 27:S:49:VAL:HB    | 27:S:115:LYS:HB3  | 1.80                     | 0.62              |
| 32:a:60:GLU:HG2   | 32:a:69:TRP:HD1   | 1.64                     | 0.62              |
| 46:r:183:ARG:HH12 | 51:w:53:A:H1'     | 1.64                     | 0.62              |
| 20:L:182:CYS:SG   | 20:L:183:LYS:N    | 2.73                     | 0.62              |
| 40:k:138:ARG:HB2  | 40:k:150:PHE:H    | 1.64                     | 0.62              |
| 9:A:999:G:O6      | 25:Q:15:ARG:HA    | 1.99                     | 0.62              |
| 46:r:4:LEU:HB2    | 46:r:124:ASP:HB3  | 1.82                     | 0.61              |
| 9:A:1550:G:H3'    | 9:A:1579:A:H61    | 1.65                     | 0.61              |
| 9:A:21:U:O2'      | 12:D:17:ARG:O     | 2.17                     | 0.61              |
| 9:A:1513:C:H5''   | 39:i:9:SER:CB     | 2.31                     | 0.61              |
| 9:A:377:G:H5'     | 26:R:98:LYS:HD3   | 1.82                     | 0.61              |
| 19:K:17:CYS:SG    | 19:K:18:SER:N     | 2.73                     | 0.61              |
| 24:P:99:ALA:H     | 24:P:133:THR:HG22 | 1.64                     | 0.61              |
| 37:f:13:LEU:HB2   | 37:f:20:ILE:HB    | 1.82                     | 0.61              |
| 9:A:1016:U:C2     | 17:I:17:PRO:CD    | 2.83                     | 0.61              |
| 11:C:95:THR:HG22  | 28:T:16:ARG:HB2   | 1.81                     | 0.61              |
| 45:q:35:TYR:CD2   | 45:q:108:GLU:HB2  | 2.35                     | 0.61              |
| 9:A:821:G:C6      | 12:D:150:ARG:HG3  | 2.35                     | 0.61              |
| 11:C:229:GLY:HA3  | 11:C:234:PRO:HA   | 1.82                     | 0.61              |
| 1:1:319:PHE:HA    | 1:1:329:ILE:H     | 1.65                     | 0.61              |
| 9:A:1752:C:O2'    | 9:A:1782:G:N2     | 2.34                     | 0.61              |
| 26:R:101:ILE:HD12 | 26:R:190:LEU:HD11 | 1.83                     | 0.61              |
| 27:S:58:LYS:HA    | 27:S:107:SER:HB2  | 1.83                     | 0.61              |
| 49:u:482:VAL:O    | 53:y:798:VAL:HG23 | 2.01                     | 0.61              |
| 50:v:247:GLN:HG2  | 50:v:250:CYS:HB2  | 1.82                     | 0.61              |
| 9:A:1488:C:O2'    | 9:A:1490:G:OP2    | 2.17                     | 0.61              |
| 9:A:1556:A:C2     | 39:i:13:LYS:HA    | 2.36                     | 0.61              |
| 9:A:1565:C:H5     | 35:d:101:ARG:NH1  | 1.99                     | 0.61              |
| 9:A:1849:G:H4'    | 44:p:65:LYS:HD3   | 1.82                     | 0.61              |
| 9:A:1613:G:OP2    | 33:b:39:ALA:N     | 2.31                     | 0.60              |
| 36:e:51:ASP:OD1   | 36:e:51:ASP:N     | 2.31                     | 0.60              |
| 49:u:230:LEU:HD12 | 49:u:256:ILE:HG23 | 1.83                     | 0.60              |
| 34:c:165:ILE:HB   | 34:c:177:TRP:HB2  | 1.83                     | 0.60              |
| 9:A:570:C:O2      | 28:T:34:THR:HB    | 2.01                     | 0.60              |
| 9:A:1396:A:O2'    | 9:A:1398:G:N7     | 2.31                     | 0.60              |
| 22:N:147:LEU:O    | 22:N:165:ASN:ND2  | 2.34                     | 0.60              |
| 36:e:101:SER:HB3  | 36:e:108:ILE:HD12 | 1.82                     | 0.60              |
| 1:1:546:ILE:HB    | 1:1:557:ASP:HB2   | 1.83                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:C:68:ARG:HE    | 11:C:76:VAL:HG11  | 1.66                     | 0.60              |
| 24:P:40:THR:HG23  | 24:P:58:GLY:HA3   | 1.81                     | 0.60              |
| 24:P:66:ARG:HH12  | 46:r:53:ARG:CB    | 2.11                     | 0.60              |
| 37:f:85:ASN:HD22  | 37:f:98:VAL:HG23  | 1.65                     | 0.60              |
| 9:A:535:G:N2      | 9:A:536:A:N7      | 2.49                     | 0.60              |
| 21:M:35:CYS:HA    | 21:M:38:ILE:HG12  | 1.84                     | 0.60              |
| 41:m:26:LEU:HD22  | 41:m:90:GLY:HA3   | 1.84                     | 0.60              |
| 9:A:521:A:OP1     | 12:D:45:ARG:NH1   | 2.35                     | 0.60              |
| 16:H:79:PHE:O     | 52:x:79:SER:N     | 2.33                     | 0.60              |
| 39:i:7:TYR:O      | 39:i:8:TRP:C      | 2.43                     | 0.60              |
| 33:b:118:GLU:O    | 37:f:119:ALA:HA   | 2.02                     | 0.60              |
| 41:m:61:TYR:CZ    | 41:m:107:SER:HB2  | 2.37                     | 0.60              |
| 3:4:304:VAL:C     | 49:u:538:LYS:HG2  | 2.26                     | 0.60              |
| 9:A:1281:G:H2'    | 9:A:1282:A:C8     | 2.37                     | 0.60              |
| 21:M:17:ILE:HD11  | 21:M:69:ILE:HD13  | 1.82                     | 0.60              |
| 40:k:135:HIS:HB2  | 40:k:140:TYR:HB3  | 1.84                     | 0.60              |
| 53:y:52:ALA:HA    | 53:y:55:LYS:HE2   | 1.82                     | 0.60              |
| 9:A:686:U:OP1     | 18:J:32:LYS:N     | 2.32                     | 0.60              |
| 11:C:192:ILE:HD13 | 11:C:238:LEU:HD22 | 1.84                     | 0.60              |
| 9:A:65:C:N4       | 27:S:134:GLY:O    | 2.32                     | 0.60              |
| 50:v:372:VAL:HG23 | 50:v:384:ILE:HD13 | 1.83                     | 0.59              |
| 11:C:137:PRO:HG2  | 11:C:149:TYR:HA   | 1.83                     | 0.59              |
| 33:b:108:LYS:NZ   | 37:f:116:LYS:HG2  | 2.16                     | 0.59              |
| 43:o:273:ASP:HA   | 43:o:280:LYS:HE2  | 1.84                     | 0.59              |
| 44:p:56:LYS:HA    | 44:p:59:LEU:HD21  | 1.83                     | 0.59              |
| 51:w:3:C:H42      | 51:w:69:G:H1      | 1.49                     | 0.59              |
| 9:A:926:A:H61     | 9:A:1015:U:H3     | 1.49                     | 0.59              |
| 1:1:659:TRP:HA    | 1:1:666:VAL:HA    | 1.82                     | 0.59              |
| 9:A:389:A:H4'     | 26:R:87:ASN:ND2   | 2.18                     | 0.59              |
| 9:A:1214:A:H2'    | 9:A:1217:A:N7     | 2.16                     | 0.59              |
| 10:B:47:PRO:HB2   | 10:B:50:ALA:H     | 1.67                     | 0.59              |
| 19:K:9:VAL:HG21   | 20:L:177:PRO:CD   | 2.33                     | 0.59              |
| 21:M:20:TYR:HE1   | 21:M:23:ARG:HH21  | 1.48                     | 0.59              |
| 40:k:135:HIS:HB2  | 40:k:140:TYR:CB   | 2.33                     | 0.59              |
| 41:m:87:GLU:HA    | 41:m:92:CYS:HB3   | 1.84                     | 0.59              |
| 46:r:183:ARG:NH1  | 51:w:53:A:H1'     | 2.17                     | 0.59              |
| 48:t:442:ALA:HA   | 48:t:456:TRP:HA   | 1.84                     | 0.59              |
| 4:5:206:LYS:HA    | 4:5:269:LEU:H     | 1.67                     | 0.59              |
| 9:A:447:A:OP1     | 26:R:49:ARG:NH1   | 2.36                     | 0.59              |
| 26:R:87:ASN:HB3   | 26:R:90:LEU:HG    | 1.84                     | 0.59              |
| 29:V:102:LEU:HD21 | 36:e:100:VAL:HG21 | 1.84                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 49:u:137:THR:HA   | 49:u:140:ARG:HG3  | 1.84                     | 0.59              |
| 5:6:351:TYR:O     | 5:6:355:ASN:ND2   | 2.34                     | 0.59              |
| 9:A:618:C:OP1     | 13:E:87:ASN:HA    | 2.03                     | 0.59              |
| 11:C:177:THR:HA   | 11:C:195:ILE:HB   | 1.85                     | 0.59              |
| 45:q:36:ALA:H     | 45:q:52:PHE:HB3   | 1.67                     | 0.59              |
| 9:A:1416:C:H4'    | 35:d:132:ASP:CB   | 2.33                     | 0.59              |
| 39:i:21:CYS:HB3   | 39:i:26:ASN:H     | 1.68                     | 0.59              |
| 49:u:51:MET:HB3   | 49:u:89:VAL:HG21  | 1.83                     | 0.59              |
| 9:A:1122:A:H4'    | 23:O:205:TYR:CE2  | 2.38                     | 0.59              |
| 9:A:1380:C:H1'    | 22:N:113:GLN:NE2  | 2.17                     | 0.59              |
| 9:A:1417:C:H1'    | 35:d:3:GLY:HA2    | 1.85                     | 0.59              |
| 9:A:1822:A:H3'    | 9:A:1823:A:C8     | 2.38                     | 0.59              |
| 9:A:379:C:H5'     | 26:R:33:ALA:HA    | 1.85                     | 0.58              |
| 35:d:35:ASP:N     | 35:d:35:ASP:OD1   | 2.36                     | 0.58              |
| 45:q:27:VAL:HG22  | 45:q:30:GLU:HG3   | 1.84                     | 0.58              |
| 50:v:246:ILE:HD11 | 52:x:26:ARG:HH12  | 1.68                     | 0.58              |
| 9:A:2:A:N7        | 20:L:223:TYR:CD2  | 2.71                     | 0.58              |
| 27:S:67:VAL:HB    | 27:S:99:GLY:HA2   | 1.84                     | 0.58              |
| 49:u:307:ARG:HD2  | 49:u:309:ASN:HB2  | 1.85                     | 0.58              |
| 9:A:307:G:N1      | 26:R:44:HIS:CG    | 2.71                     | 0.58              |
| 29:V:102:LEU:HD11 | 36:e:100:VAL:CG2  | 2.31                     | 0.58              |
| 53:y:570:LEU:HD22 | 53:y:612:THR:HG21 | 1.85                     | 0.58              |
| 9:A:888:U:H3      | 9:A:900:C:H42     | 1.49                     | 0.58              |
| 9:A:1441:U:O2     | 9:A:1443:C:N4     | 2.36                     | 0.58              |
| 49:u:124:PRO:HA   | 49:u:127:VAL:HG22 | 1.85                     | 0.58              |
| 9:A:570:C:O2'     | 28:T:34:THR:O     | 2.18                     | 0.58              |
| 23:O:175:GLU:O    | 23:O:179:ASN:ND2  | 2.37                     | 0.58              |
| 22:N:84:GLN:HG2   | 22:N:100:ALA:HB1  | 1.84                     | 0.58              |
| 49:u:487:THR:HA   | 53:y:840:GLN:HE22 | 1.69                     | 0.58              |
| 52:x:307:ASN:HA   | 52:x:312:LEU:HD13 | 1.86                     | 0.58              |
| 9:A:1679:A:C2     | 29:V:60:ARG:HG3   | 2.39                     | 0.58              |
| 23:O:75:GLN:NE2   | 49:u:17:GLU:OE2   | 2.37                     | 0.58              |
| 23:O:139:CYS:SG   | 23:O:140:VAL:N    | 2.77                     | 0.58              |
| 29:V:48:TYR:HB3   | 30:Y:49:TYR:HB3   | 1.86                     | 0.58              |
| 49:u:481:GLN:O    | 49:u:494:GLY:N    | 2.37                     | 0.58              |
| 9:A:1757:G:H8     | 9:A:1777:G:H1     | 1.52                     | 0.58              |
| 50:v:220:PHE:O    | 50:v:229:ARG:NH2  | 2.36                     | 0.58              |
| 9:A:868:G:H2'     | 15:G:115:LYS:HE2  | 1.86                     | 0.57              |
| 9:A:1377:U:C2     | 22:N:102:ARG:NH2  | 2.72                     | 0.57              |
| 15:G:154:ILE:HB   | 15:G:185:VAL:HG12 | 1.86                     | 0.57              |
| 9:A:1308:U:H4'    | 40:k:133:ALA:HA   | 1.85                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:A:1713:C:OP1    | 13:E:71:ARG:NH2   | 2.37                     | 0.57              |
| 28:T:80:ASP:OD1   | 28:T:80:ASP:N     | 2.37                     | 0.57              |
| 31:Z:20:GLU:HG3   | 32:a:64:TRP:CG    | 2.39                     | 0.57              |
| 47:s:176:TYR:HA   | 47:s:179:LEU:HD12 | 1.85                     | 0.57              |
| 1:1:481:PHE:HB2   | 1:1:494:THR:HB    | 1.86                     | 0.57              |
| 9:A:588:G:H4'     | 9:A:589:G:H5'     | 1.86                     | 0.57              |
| 9:A:919:A:H5''    | 17:I:16:LEU:HD12  | 1.85                     | 0.57              |
| 9:A:1598:G:O6     | 36:e:85:ARG:NH1   | 2.37                     | 0.57              |
| 9:A:1679:A:C2'    | 29:V:60:ARG:HD2   | 2.34                     | 0.57              |
| 30:Y:45:ARG:HA    | 30:Y:48:GLN:HB2   | 1.85                     | 0.57              |
| 33:b:108:LYS:HB2  | 33:b:111:MET:HE3  | 1.86                     | 0.57              |
| 34:c:90:TRP:HA    | 34:c:97:THR:HA    | 1.87                     | 0.57              |
| 21:M:76:GLU:O     | 21:M:80:ARG:N     | 2.37                     | 0.57              |
| 9:A:1674:G:H4'    | 29:V:77:MET:HE1   | 1.85                     | 0.57              |
| 44:p:39:ASN:H     | 44:p:42:LYS:HB2   | 1.70                     | 0.57              |
| 9:A:1245:G:H2'    | 9:A:1246:A:C8     | 2.39                     | 0.57              |
| 9:A:1335:G:H4'    | 31:Z:172:VAL:HG11 | 1.87                     | 0.57              |
| 10:B:86:ILE:HG23  | 10:B:113:LEU:HB2  | 1.87                     | 0.57              |
| 39:i:38:MET:HE1   | 39:i:50:ILE:HD11  | 1.86                     | 0.57              |
| 52:x:31:GLN:OE1   | 52:x:67:SER:N     | 2.37                     | 0.57              |
| 1:1:478:ILE:HD12  | 1:1:497:GLN:HG2   | 1.87                     | 0.57              |
| 3:4:341:ALA:HB1   | 7:8:329:ASN:HA    | 1.87                     | 0.57              |
| 9:A:1513:C:H5''   | 39:i:9:SER:HB3    | 1.87                     | 0.57              |
| 13:E:105:PHE:HB3  | 13:E:112:VAL:HG21 | 1.87                     | 0.57              |
| 18:J:80:ASP:OD1   | 18:J:80:ASP:N     | 2.38                     | 0.57              |
| 22:N:80:ARG:NH2   | 22:N:82:THR:OG1   | 2.38                     | 0.57              |
| 1:1:437:PHE:HA    | 1:1:451:THR:H     | 1.69                     | 0.57              |
| 24:P:67:ASP:OD2   | 46:r:53:ARG:NH1   | 2.37                     | 0.57              |
| 30:Y:143:LYS:HD3  | 30:Y:145:TYR:CZ   | 2.39                     | 0.57              |
| 45:q:34:GLU:HB2   | 45:q:52:PHE:CG    | 2.39                     | 0.57              |
| 47:s:212:VAL:HG13 | 47:s:216:LYS:HE3  | 1.87                     | 0.57              |
| 49:u:417:GLN:HB3  | 49:u:420:LYS:HB3  | 1.87                     | 0.57              |
| 7:8:31:SER:HA     | 7:8:37:LYS:HA     | 1.86                     | 0.57              |
| 9:A:65:C:C6       | 27:S:174:PRO:HB3  | 2.40                     | 0.57              |
| 9:A:688:U:C6      | 15:G:122:LEU:HD13 | 2.40                     | 0.57              |
| 9:A:1122:A:H5''   | 23:O:205:TYR:CE2  | 2.40                     | 0.57              |
| 9:A:1203:G:H2'    | 9:A:1204:A:C8     | 2.39                     | 0.57              |
| 9:A:1824:A:H1'    | 45:q:45:GLY:HA3   | 1.86                     | 0.57              |
| 24:P:54:CYS:SG    | 24:P:55:ARG:N     | 2.78                     | 0.57              |
| 36:e:48:VAL:HG11  | 37:f:23:ARG:HA    | 1.86                     | 0.57              |
| 9:A:681:U:H4'     | 13:E:9:THR:HG22   | 1.85                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:A:1016:U:C5     | 16:H:28:PRO:HG3   | 2.39                     | 0.56              |
| 9:A:1219:C:H2'    | 9:A:1220:A:C8     | 2.39                     | 0.56              |
| 9:A:1656:G:H1     | 9:A:1668:U:H3     | 1.53                     | 0.56              |
| 40:k:141:CYS:HB3  | 40:k:144:CYS:CB   | 2.35                     | 0.56              |
| 9:A:1199:A:OP1    | 25:Q:2:THR:N      | 2.38                     | 0.56              |
| 50:v:208:LEU:HD21 | 50:v:246:ILE:HB   | 1.87                     | 0.56              |
| 9:A:380:G:H5''    | 26:R:31:ARG:NH1   | 2.20                     | 0.56              |
| 9:A:546:G:N2      | 9:A:547:G:O6      | 2.37                     | 0.56              |
| 9:A:1077:A:O2'    | 53:y:51:SER:CB    | 2.52                     | 0.56              |
| 9:A:1232:U:H2'    | 9:A:1233:G:C8     | 2.41                     | 0.56              |
| 9:A:1275:G:O4'    | 9:A:1506:A:N6     | 2.38                     | 0.56              |
| 9:A:1524:G:N7     | 37:f:141:ARG:NH1  | 2.51                     | 0.56              |
| 9:A:1680:G:O2'    | 42:n:20:ARG:HD3   | 2.06                     | 0.56              |
| 23:O:72:ALA:HB3   | 24:P:128:ARG:HH12 | 1.70                     | 0.56              |
| 29:V:71:ARG:NH1   | 29:V:148:ASN:OD1  | 2.38                     | 0.56              |
| 30:Y:42:ILE:HG22  | 30:Y:44:PRO:HD2   | 1.88                     | 0.56              |
| 31:Z:55:THR:HG21  | 31:Z:89:GLU:C     | 2.30                     | 0.56              |
| 41:m:32:ALA:HB3   | 41:m:110:VAL:HB   | 1.88                     | 0.56              |
| 9:A:917:U:O4'     | 15:G:118:ARG:HG2  | 2.05                     | 0.56              |
| 32:a:49:MET:HG3   | 32:a:69:TRP:CD2   | 2.40                     | 0.56              |
| 9:A:1615:U:H3     | 33:b:40:ARG:HH22  | 1.54                     | 0.56              |
| 22:N:140:VAL:HG13 | 22:N:142:LEU:HG   | 1.88                     | 0.56              |
| 24:P:117:ARG:HD2  | 25:Q:49:ALA:HB2   | 1.87                     | 0.56              |
| 36:e:82:SER:OG    | 37:f:55:ARG:NH1   | 2.39                     | 0.56              |
| 37:f:27:ALA:HB2   | 37:f:52:LEU:HD22  | 1.85                     | 0.56              |
| 46:r:200:TYR:CD1  | 48:t:343:ILE:HA   | 2.40                     | 0.56              |
| 47:s:212:VAL:HG23 | 47:s:214:THR:H    | 1.69                     | 0.56              |
| 11:C:48:LEU:HD12  | 11:C:61:VAL:HG13  | 1.87                     | 0.56              |
| 19:K:43:THR:HG1   | 19:K:45:ARG:HH21  | 1.53                     | 0.56              |
| 9:A:1535:U:O4     | 29:V:159:ARG:NH1  | 2.39                     | 0.56              |
| 37:f:98:VAL:HG11  | 37:f:106:LYS:HG3  | 1.87                     | 0.56              |
| 49:u:319:SER:HB3  | 49:u:379:VAL:HB   | 1.87                     | 0.56              |
| 5:6:324:LYS:O     | 49:u:448:GLN:HG3  | 2.06                     | 0.56              |
| 9:A:562:U:H4'     | 12:D:132:GLN:HB3  | 1.88                     | 0.56              |
| 9:A:1154:U:O2'    | 20:L:185:THR:HG21 | 2.06                     | 0.56              |
| 9:A:1350:U:H1'    | 22:N:110:ASN:OD1  | 2.06                     | 0.56              |
| 27:S:23:LYS:HD3   | 27:S:41:LEU:HA    | 1.88                     | 0.56              |
| 3:4:111:GLU:HA    | 49:u:577:GLU:CB   | 2.36                     | 0.56              |
| 9:A:570:C:O3'     | 28:T:36:PRO:HA    | 2.06                     | 0.56              |
| 9:A:973:C:N3      | 24:P:55:ARG:NH2   | 2.54                     | 0.56              |
| 9:A:1016:U:C2     | 17:I:17:PRO:HD3   | 2.41                     | 0.56              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 9:A:1593:C:O2    | 35:d:12:GLN:NE2   | 2.32                     | 0.56              |
| 9:A:1679:A:N3    | 29:V:60:ARG:HG3   | 2.21                     | 0.56              |
| 16:H:65:GLN:HG3  | 53:y:341:GLY:O    | 2.06                     | 0.56              |
| 21:M:78:ARG:HD3  | 22:N:89:LYS:HZ1   | 1.70                     | 0.56              |
| 45:q:80:GLY:N    | 45:q:90:ASP:O     | 2.37                     | 0.56              |
| 49:u:561:SER:O   | 49:u:565:HIS:N    | 2.39                     | 0.56              |
| 50:v:303:PHE:HE1 | 53:y:824:LYS:HD2  | 1.70                     | 0.56              |
| 9:A:1292:C:C6    | 40:k:142:GLY:HA2  | 2.40                     | 0.56              |
| 46:r:52:SER:HA   | 46:r:88:ARG:HB3   | 1.87                     | 0.56              |
| 49:u:300:TYR:HD2 | 49:u:376:ARG:HH12 | 1.54                     | 0.55              |
| 50:v:302:ASN:HB2 | 53:y:820:SER:HB2  | 1.88                     | 0.55              |
| 9:A:1335:G:H4'   | 31:Z:172:VAL:CG1  | 2.36                     | 0.55              |
| 9:A:1849:G:OP1   | 44:p:61:LYS:HG2   | 2.06                     | 0.55              |
| 12:D:113:GLN:OE1 | 12:D:154:GLN:NE2  | 2.38                     | 0.55              |
| 17:I:16:LEU:N    | 18:J:57:ARG:HH22  | 2.04                     | 0.55              |
| 34:c:79:LEU:HD11 | 34:c:87:LEU:HD23  | 1.89                     | 0.55              |
| 39:i:7:TYR:O     | 39:i:9:SER:N      | 2.38                     | 0.55              |
| 41:m:92:CYS:HA   | 41:m:103:VAL:HG23 | 1.88                     | 0.55              |
| 53:y:735:GLU:HA  | 53:y:738:VAL:HG12 | 1.88                     | 0.55              |
| 9:A:161:U:O4'    | 28:T:116:LYS:HA   | 2.05                     | 0.55              |
| 9:A:553:U:O4     | 9:A:555:A:N6      | 2.39                     | 0.55              |
| 30:Y:93:VAL:HG21 | 30:Y:120:LEU:HD21 | 1.87                     | 0.55              |
| 40:k:133:ALA:HB3 | 40:k:140:TYR:CB   | 2.35                     | 0.55              |
| 45:q:65:LEU:HD11 | 45:q:92:ILE:C     | 2.32                     | 0.55              |
| 46:r:273:MET:HE1 | 51:w:2:G:O2'      | 2.06                     | 0.55              |
| 9:A:110:U:H5''   | 11:C:205:PHE:HE1  | 1.71                     | 0.55              |
| 9:A:1230:C:HO2'  | 9:A:1665:G:H1     | 1.53                     | 0.55              |
| 19:K:16:LYS:HD3  | 20:L:259:THR:HG23 | 1.89                     | 0.55              |
| 21:M:109:LEU:CD1 | 22:N:52:LYS:HB2   | 2.36                     | 0.55              |
| 9:A:67:C:N4      | 27:S:168:LYS:O    | 2.40                     | 0.55              |
| 9:A:614:C:O2'    | 45:q:63:GLY:HA3   | 2.06                     | 0.55              |
| 9:A:921:G:C2     | 16:H:22:LYS:HG2   | 2.41                     | 0.55              |
| 9:A:948:C:H2'    | 9:A:949:G:H8      | 1.70                     | 0.55              |
| 19:K:29:HIS:CG   | 20:L:87:PRO:HB3   | 2.42                     | 0.55              |
| 19:K:56:CYS:SG   | 19:K:57:GLY:N     | 2.78                     | 0.55              |
| 21:M:30:THR:O    | 21:M:34:VAL:HG23  | 2.07                     | 0.55              |
| 34:c:272:GLN:NE2 | 34:c:284:PRO:O    | 2.40                     | 0.55              |
| 42:n:38:THR:HA   | 52:x:426:LYS:HE2  | 1.89                     | 0.55              |
| 1:1:617:SER:HA   | 1:1:659:TRP:CB    | 2.37                     | 0.55              |
| 9:A:4:C:O5'      | 20:L:207:ALA:HB2  | 2.06                     | 0.55              |
| 9:A:943:U:OP1    | 23:O:214:LYS:NZ   | 2.30                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:A:1587:G:O6     | 35:d:67:ARG:HG2   | 2.06                     | 0.55              |
| 53:y:358:VAL:HG21 | 53:y:378:ILE:HD11 | 1.88                     | 0.55              |
| 3:4:263:ILE:O     | 3:4:265:LEU:N     | 2.39                     | 0.55              |
| 9:A:307:G:O6      | 26:R:44:HIS:NE2   | 2.39                     | 0.55              |
| 21:M:111:PHE:CE2  | 22:N:15:VAL:HG21  | 2.42                     | 0.55              |
| 41:m:95:ASP:HB3   | 41:m:101:ARG:HE   | 1.72                     | 0.55              |
| 53:y:781:ARG:HH11 | 53:y:817:THR:HG21 | 1.72                     | 0.55              |
| 9:A:982:G:H2'     | 9:A:983:A:C8      | 2.42                     | 0.55              |
| 9:A:1648:G:H5''   | 30:Y:125:ARG:CB   | 2.36                     | 0.55              |
| 20:L:168:GLY:N    | 20:L:179:THR:O    | 2.37                     | 0.55              |
| 27:S:44:GLU:HG3   | 27:S:45:TRP:HD1   | 1.72                     | 0.55              |
| 37:f:20:ILE:HD13  | 37:f:30:ILE:HG22  | 1.89                     | 0.55              |
| 49:u:91:ARG:HH21  | 49:u:173:LEU:HD22 | 1.72                     | 0.55              |
| 2:3:36:GLN:HA     | 2:3:41:ALA:HB3    | 1.89                     | 0.55              |
| 9:A:841:G:OP2     | 28:T:14:THR:HB    | 2.07                     | 0.55              |
| 16:H:3:LEU:N      | 19:K:64:GLU:OE1   | 2.37                     | 0.55              |
| 32:a:23:ALA:HB3   | 32:a:69:TRP:HH2   | 1.72                     | 0.55              |
| 32:a:32:HIS:HE1   | 32:a:34:GLU:HB2   | 1.72                     | 0.55              |
| 46:r:86:SER:OG    | 46:r:87:LYS:N     | 2.38                     | 0.55              |
| 9:A:537:C:O2      | 9:A:546:G:N2      | 2.39                     | 0.55              |
| 34:c:20:GLN:HG2   | 34:c:69:VAL:H     | 1.72                     | 0.55              |
| 34:c:146:SER:OG   | 34:c:147:HIS:N    | 2.40                     | 0.55              |
| 49:u:286:SER:HA   | 53:y:728:GLY:HA2  | 1.89                     | 0.55              |
| 52:x:44:ASP:OD1   | 52:x:47:GLY:N     | 2.38                     | 0.55              |
| 29:V:127:ARG:HH21 | 42:n:24:GLN:HE22  | 1.53                     | 0.54              |
| 31:Z:67:ARG:NH1   | 32:a:96:ARG:H     | 2.05                     | 0.54              |
| 31:Z:99:ILE:HG23  | 31:Z:173:ARG:NH2  | 2.23                     | 0.54              |
| 34:c:107:ASP:N    | 34:c:107:ASP:OD1  | 2.40                     | 0.54              |
| 9:A:1473:G:N1     | 9:A:1476:A:OP2    | 2.38                     | 0.54              |
| 9:A:1565:C:OP2    | 35:d:101:ARG:NE   | 2.37                     | 0.54              |
| 9:A:1619:A:OP1    | 33:b:47:ARG:NE    | 2.34                     | 0.54              |
| 15:G:117:PRO:HB2  | 15:G:120:ARG:HG3  | 1.87                     | 0.54              |
| 1:1:307:SER:HA    | 1:1:319:PHE:CB    | 2.37                     | 0.54              |
| 9:A:798:G:C5      | 15:G:107:LYS:C    | 2.85                     | 0.54              |
| 9:A:1357:A:OP1    | 20:L:125:LYS:NZ   | 2.36                     | 0.54              |
| 9:A:1579:A:OP2    | 31:Z:7:LYS:HG2    | 2.08                     | 0.54              |
| 34:c:88:ARG:HH11  | 34:c:97:THR:HG21  | 1.71                     | 0.54              |
| 52:x:76:ASP:N     | 52:x:76:ASP:OD1   | 2.39                     | 0.54              |
| 9:A:77:A:O2'      | 27:S:174:PRO:O    | 2.24                     | 0.54              |
| 9:A:818:A:OP1     | 12:D:80:ARG:NH2   | 2.37                     | 0.54              |
| 21:M:20:TYR:HE1   | 21:M:23:ARG:NH2   | 2.05                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 29:V:34:SER:HA    | 42:n:55:VAL:HB    | 1.89                     | 0.54              |
| 33:b:111:MET:HB3  | 37:f:117:ILE:HD11 | 1.89                     | 0.54              |
| 35:d:73:GLY:O     | 35:d:94:ARG:NH1   | 2.41                     | 0.54              |
| 45:q:97:ALA:HA    | 45:q:100:ALA:HB3  | 1.90                     | 0.54              |
| 9:A:380:G:OP1     | 26:R:31:ARG:NH1   | 2.30                     | 0.54              |
| 9:A:1308:U:H4'    | 40:k:133:ALA:CB   | 2.38                     | 0.54              |
| 11:C:213:ALA:HB3  | 11:C:244:ILE:HD11 | 1.90                     | 0.54              |
| 31:Z:109:LEU:HD12 | 31:Z:184:ILE:HD11 | 1.90                     | 0.54              |
| 44:p:75:GLU:HG3   | 44:p:81:GLU:HG3   | 1.89                     | 0.54              |
| 49:u:201:LEU:O    | 49:u:233:ARG:NH2  | 2.40                     | 0.54              |
| 53:y:358:VAL:HG22 | 53:y:374:ILE:HG13 | 1.89                     | 0.54              |
| 9:A:2:A:N7        | 20:L:223:TYR:CE2  | 2.76                     | 0.54              |
| 9:A:925:G:OP1     | 17:I:121:ARG:NH2  | 2.40                     | 0.54              |
| 20:L:76:LYS:NZ    | 20:L:80:GLU:OE1   | 2.41                     | 0.54              |
| 31:Z:166:TYR:O    | 31:Z:200:PRO:HG3  | 2.07                     | 0.54              |
| 50:v:263:THR:HG21 | 50:v:328:CYS:HB2  | 1.90                     | 0.54              |
| 9:A:1545:A:OP1    | 30:Y:74:GLY:N     | 2.35                     | 0.54              |
| 34:c:28:PRO:O     | 34:c:47:ARG:NH1   | 2.40                     | 0.54              |
| 48:t:85:ASN:HA    | 48:t:131:SER:HA   | 1.90                     | 0.54              |
| 2:3:151:GLN:O     | 2:3:189:ILE:N     | 2.41                     | 0.54              |
| 9:A:1248:U:C2     | 51:w:33:C:H4'     | 2.43                     | 0.54              |
| 9:A:1708:C:H2'    | 9:A:1709:G:H8     | 1.73                     | 0.54              |
| 23:O:32:ASP:HA    | 23:O:46:LYS:HA    | 1.90                     | 0.54              |
| 28:T:45:ALA:HB1   | 28:T:50:THR:O     | 2.08                     | 0.54              |
| 29:V:204:ARG:HG2  | 42:n:63:ARG:NH2   | 2.22                     | 0.54              |
| 30:Y:13:PHE:HA    | 30:Y:22:VAL:HA    | 1.90                     | 0.54              |
| 9:A:307:G:C6      | 26:R:44:HIS:CG    | 2.96                     | 0.54              |
| 49:u:548:GLU:O    | 49:u:552:LEU:N    | 2.37                     | 0.54              |
| 4:5:210:GLU:O     | 4:5:214:PHE:N     | 2.41                     | 0.54              |
| 9:A:1299:A:O2'    | 33:b:52:LYS:HE2   | 2.07                     | 0.54              |
| 45:q:79:VAL:HA    | 45:q:91:VAL:HA    | 1.89                     | 0.54              |
| 50:v:262:ILE:O    | 50:v:335:ASN:ND2  | 2.40                     | 0.54              |
| 1:1:612:ASN:H     | 1:1:627:GLY:HA2   | 1.73                     | 0.53              |
| 2:3:170:LEU:O     | 2:3:174:MET:N     | 2.38                     | 0.53              |
| 9:A:1124:C:H5''   | 23:O:150:ILE:HG12 | 1.89                     | 0.53              |
| 9:A:1291:A:H1'    | 40:k:143:LYS:HB2  | 1.90                     | 0.53              |
| 9:A:585:C:H2'     | 9:A:586:G:C8      | 2.43                     | 0.53              |
| 9:A:1237:C:O2'    | 9:A:1522:A:N1     | 2.41                     | 0.53              |
| 9:A:1631:U:H5''   | 37:f:34:LYS:HG3   | 1.89                     | 0.53              |
| 31:Z:59:LEU:HD12  | 31:Z:66:ILE:HG13  | 1.89                     | 0.53              |
| 5:6:324:LYS:HB2   | 49:u:447:TYR:HA   | 1.89                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:A:869:A:N6      | 15:G:117:PRO:HG3  | 2.23                     | 0.53              |
| 9:A:996:A:OP1     | 17:I:114:ARG:NH1  | 2.37                     | 0.53              |
| 9:A:1630:A:OP1    | 37:f:37:GLY:HA3   | 2.09                     | 0.53              |
| 21:M:106:LEU:HB3  | 21:M:111:PHE:HB2  | 1.90                     | 0.53              |
| 30:Y:25:CYS:HB2   | 30:Y:68:ILE:HG12  | 1.90                     | 0.53              |
| 41:m:93:LYS:H     | 41:m:103:VAL:HA   | 1.74                     | 0.53              |
| 49:u:109:GLN:HA   | 49:u:112:VAL:HG12 | 1.91                     | 0.53              |
| 9:A:1416:C:O2'    | 35:d:4:VAL:O      | 2.26                     | 0.53              |
| 9:A:1863:A:H1'    | 25:Q:79:ILE:HD11  | 1.91                     | 0.53              |
| 12:D:33:GLY:HA3   | 14:F:112:TYR:CG   | 2.42                     | 0.53              |
| 16:H:30:SER:OG    | 16:H:31:TYR:N     | 2.40                     | 0.53              |
| 23:O:70:SER:OG    | 23:O:71:LEU:N     | 2.42                     | 0.53              |
| 24:P:116:LEU:HD11 | 25:Q:45:VAL:CG1   | 2.39                     | 0.53              |
| 44:p:112:GLY:HA3  | 47:s:273:ARG:HH22 | 1.73                     | 0.53              |
| 50:v:375:ILE:HB   | 50:v:384:ILE:HD11 | 1.91                     | 0.53              |
| 9:A:380:G:P       | 26:R:56:ARG:HH22  | 2.32                     | 0.53              |
| 15:G:184:ASP:OD1  | 15:G:184:ASP:N    | 2.41                     | 0.53              |
| 25:Q:25:ASN:ND2   | 25:Q:77:CYS:SG    | 2.82                     | 0.53              |
| 53:y:333:LEU:HD13 | 53:y:374:ILE:HG22 | 1.90                     | 0.53              |
| 1:1:544:PHE:HB2   | 1:1:559:VAL:HB    | 1.91                     | 0.53              |
| 9:A:307:G:C2      | 26:R:44:HIS:HB3   | 2.43                     | 0.53              |
| 9:A:563:G:HO2'    | 9:A:564:A:H8      | 1.56                     | 0.53              |
| 9:A:574:A:H4'     | 28:T:89:HIS:CB    | 2.39                     | 0.53              |
| 9:A:957:A:OP1     | 24:P:57:THR:HG21  | 2.08                     | 0.53              |
| 38:h:69:PRO:HA    | 39:i:41:GLN:NE2   | 2.24                     | 0.53              |
| 49:u:270:GLN:HB2  | 49:u:306:MET:HE1  | 1.90                     | 0.53              |
| 49:u:337:ASP:N    | 49:u:337:ASP:OD1  | 2.41                     | 0.53              |
| 49:u:476:ARG:NH1  | 53:y:794:THR:OG1  | 2.41                     | 0.53              |
| 49:u:558:LEU:O    | 49:u:562:ARG:N    | 2.42                     | 0.53              |
| 52:x:169:GLU:O    | 52:x:521:SER:N    | 2.41                     | 0.53              |
| 9:A:685:A:H5''    | 18:J:31:SER:HB3   | 1.89                     | 0.53              |
| 9:A:790:C:OP1     | 9:A:791:C:O2'     | 2.24                     | 0.53              |
| 9:A:1377:U:N3     | 22:N:102:ARG:NH2  | 2.57                     | 0.53              |
| 41:m:24:THR:HA    | 41:m:27:ILE:HG12  | 1.90                     | 0.53              |
| 1:1:682:TRP:HA    | 1:1:693:LYS:HA    | 1.90                     | 0.53              |
| 9:A:1657:G:H1     | 9:A:1667:U:H3     | 1.56                     | 0.53              |
| 21:M:17:ILE:O     | 21:M:18:GLU:C     | 2.52                     | 0.53              |
| 27:S:74:ARG:NH1   | 27:S:96:SER:OG    | 2.40                     | 0.53              |
| 48:t:167:GLN:O    | 48:t:169:GLN:N    | 2.36                     | 0.53              |
| 53:y:468:GLU:HA   | 53:y:471:GLU:HB2  | 1.91                     | 0.53              |
| 1:1:518:HIS:HB2   | 1:1:527:CYS:HB2   | 1.91                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:N:184:ARG:HH11 | 22:N:191:ARG:HD3  | 1.74                     | 0.53              |
| 31:Z:20:GLU:HG3   | 32:a:64:TRP:CB    | 2.39                     | 0.53              |
| 44:p:32:HIS:HB3   | 44:p:34:ARG:HE    | 1.73                     | 0.53              |
| 50:v:394:GLY:HA2  | 53:y:844:MET:HE1  | 1.92                     | 0.53              |
| 1:1:509:LEU:HD21  | 1:1:532:ARG:HD2   | 1.91                     | 0.52              |
| 1:1:616:TRP:HA    | 1:1:623:VAL:HA    | 1.91                     | 0.52              |
| 21:M:77:GLU:HA    | 21:M:80:ARG:CB    | 2.37                     | 0.52              |
| 29:V:122:ARG:HG3  | 42:n:59:LEU:HD13  | 1.90                     | 0.52              |
| 53:y:831:LEU:HD21 | 53:y:846:ARG:HB2  | 1.90                     | 0.52              |
| 1:1:349:LEU:O     | 1:1:360:TRP:N     | 2.41                     | 0.52              |
| 2:3:81:ASP:O      | 2:3:85:CYS:N      | 2.41                     | 0.52              |
| 9:A:575:A:OP2     | 28:T:93:ARG:NH2   | 2.39                     | 0.52              |
| 9:A:1824:A:H1'    | 45:q:45:GLY:C     | 2.33                     | 0.52              |
| 9:A:1824:A:H4'    | 45:q:66:ARG:HH22  | 1.74                     | 0.52              |
| 15:G:31:GLU:HA    | 15:G:40:LEU:HD23  | 1.91                     | 0.52              |
| 29:V:49:LEU:HD13  | 30:Y:47:LEU:HD22  | 1.92                     | 0.52              |
| 52:x:195:CYS:HA   | 52:x:359:ARG:HA   | 1.91                     | 0.52              |
| 9:A:65:C:C2       | 27:S:174:PRO:HD3  | 2.45                     | 0.52              |
| 20:L:196:ILE:HB   | 20:L:223:TYR:HB2  | 1.91                     | 0.52              |
| 21:M:77:GLU:O     | 21:M:78:ARG:C     | 2.51                     | 0.52              |
| 45:q:38:VAL:HG22  | 45:q:41:MET:HE2   | 1.91                     | 0.52              |
| 46:r:200:TYR:CE1  | 48:t:343:ILE:HA   | 2.44                     | 0.52              |
| 9:A:539:C:H41     | 9:A:542:U:H5''    | 1.74                     | 0.52              |
| 9:A:1351:G:H4'    | 22:N:109:THR:HB   | 1.91                     | 0.52              |
| 10:B:11:GLN:HB3   | 10:B:56:ILE:HG21  | 1.90                     | 0.52              |
| 12:D:170:PRO:O    | 12:D:175:ARG:NH1  | 2.42                     | 0.52              |
| 15:G:143:ARG:HH22 | 18:J:53:ILE:HG23  | 1.74                     | 0.52              |
| 34:c:67:SER:OG    | 34:c:108:VAL:O    | 2.24                     | 0.52              |
| 50:v:246:ILE:HD11 | 52:x:26:ARG:HH22  | 1.73                     | 0.52              |
| 50:v:304:ASP:N    | 50:v:304:ASP:OD1  | 2.41                     | 0.52              |
| 1:1:377:GLN:H     | 1:1:392:SER:HA    | 1.75                     | 0.52              |
| 9:A:1390:U:H2'    | 9:A:1391:C:C6     | 2.44                     | 0.52              |
| 11:C:26:VAL:HG22  | 12:D:4:ALA:HB2    | 1.92                     | 0.52              |
| 34:c:171:ASP:OD1  | 34:c:171:ASP:N    | 2.42                     | 0.52              |
| 44:p:111:HIS:C    | 47:s:273:ARG:HH12 | 2.16                     | 0.52              |
| 52:x:73:HIS:CG    | 53:y:602:ASP:HB3  | 2.45                     | 0.52              |
| 9:A:687:C:H4'     | 15:G:121:THR:HG21 | 1.92                     | 0.52              |
| 9:A:924:G:O3'     | 17:I:121:ARG:NH1  | 2.43                     | 0.52              |
| 9:A:1093:A:H5''   | 18:J:28:ARG:NH2   | 2.23                     | 0.52              |
| 9:A:1458:G:OP1    | 34:c:276:SER:OG   | 2.23                     | 0.52              |
| 11:C:175:PHE:HE2  | 11:C:198:ARG:HD2  | 1.74                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:D:18:ARG:O     | 12:D:24:ARG:NH1   | 2.42                     | 0.52              |
| 28:T:117:VAL:HG21 | 28:T:125:VAL:HG21 | 1.91                     | 0.52              |
| 30:Y:19:ALA:HB2   | 30:Y:75:GLY:HA3   | 1.90                     | 0.52              |
| 37:f:60:THR:OG1   | 37:f:61:GLU:N     | 2.42                     | 0.52              |
| 3:4:107:GLU:HA    | 49:u:568:ILE:O    | 2.10                     | 0.52              |
| 5:6:344:LYS:HG3   | 5:6:351:TYR:HE2   | 1.74                     | 0.52              |
| 9:A:373:G:H5'     | 9:A:373:G:C8      | 2.44                     | 0.52              |
| 20:L:183:LYS:HG2  | 20:L:196:ILE:HA   | 1.90                     | 0.52              |
| 38:h:80:PHE:HB3   | 39:i:52:PHE:HB3   | 1.92                     | 0.52              |
| 1:1:567:ALA:HB3   | 1:1:580:LEU:HB2   | 1.91                     | 0.52              |
| 9:A:1406:G:H21    | 9:A:1443:C:H42    | 1.55                     | 0.52              |
| 10:B:35:ARG:HD3   | 10:B:51:ILE:HA    | 1.90                     | 0.52              |
| 24:P:86:LYS:NZ    | 24:P:122:SER:O    | 2.40                     | 0.52              |
| 39:i:8:TRP:NE1    | 39:i:12:ARG:HB2   | 2.25                     | 0.52              |
| 44:p:100:ILE:HG12 | 53:y:265:GLU:CB   | 2.40                     | 0.52              |
| 49:u:443:VAL:HG22 | 49:u:447:TYR:HB2  | 1.91                     | 0.52              |
| 51:w:22:C:H2'     | 51:w:23:G:C8      | 2.45                     | 0.52              |
| 51:w:69:G:H2'     | 51:w:70:C:C6      | 2.45                     | 0.52              |
| 9:A:848:U:H2'     | 9:A:849:A:H8      | 1.75                     | 0.52              |
| 9:A:1565:C:C5     | 35:d:101:ARG:NH1  | 2.77                     | 0.52              |
| 11:C:11:ARG:NH1   | 11:C:21:ASP:H     | 2.04                     | 0.52              |
| 30:Y:95:TYR:CE1   | 30:Y:99:TYR:CD2   | 2.98                     | 0.52              |
| 43:o:300:VAL:HG22 | 43:o:310:LEU:HD11 | 1.91                     | 0.52              |
| 45:q:76:ILE:HG23  | 45:q:95:TYR:HB2   | 1.92                     | 0.52              |
| 49:u:408:THR:HA   | 49:u:411:LEU:HB2  | 1.91                     | 0.52              |
| 5:6:326:ASP:OD1   | 5:6:326:ASP:N     | 2.43                     | 0.52              |
| 9:A:482:G:N1      | 9:A:485:A:OP2     | 2.38                     | 0.52              |
| 19:K:80:SER:OG    | 19:K:81:LYS:N     | 2.43                     | 0.52              |
| 20:L:65:LYS:HG2   | 22:N:118:GLU:OE1  | 2.09                     | 0.52              |
| 34:c:124:SER:OG   | 34:c:126:ASP:OD1  | 2.27                     | 0.52              |
| 42:n:21:THR:OG1   | 42:n:22:GLY:N     | 2.43                     | 0.52              |
| 45:q:62:ARG:HD3   | 45:q:90:ASP:OD2   | 2.09                     | 0.52              |
| 47:s:231:ARG:NE   | 47:s:274:TYR:OH   | 2.43                     | 0.52              |
| 9:A:1454:A:H3'    | 21:M:5:ARG:NH1    | 2.25                     | 0.51              |
| 9:A:1708:C:H2'    | 9:A:1709:G:C8     | 2.44                     | 0.51              |
| 25:Q:2:THR:OG1    | 25:Q:3:LYS:N      | 2.42                     | 0.51              |
| 34:c:35:SER:OG    | 34:c:36:ARG:N     | 2.43                     | 0.51              |
| 34:c:83:TRP:HA    | 34:c:107:ASP:HB3  | 1.91                     | 0.51              |
| 49:u:112:VAL:HA   | 49:u:115:ILE:HB   | 1.91                     | 0.51              |
| 49:u:564:GLU:HA   | 49:u:567:ARG:HB2  | 1.91                     | 0.51              |
| 51:w:22:C:H2'     | 51:w:23:G:H8      | 1.74                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:A:534:G:N2      | 9:A:550:C:O2      | 2.43                     | 0.51              |
| 9:A:1334:G:H4'    | 31:Z:183:GLY:N    | 2.25                     | 0.51              |
| 44:p:59:LEU:HD12  | 44:p:63:PHE:CE2   | 2.45                     | 0.51              |
| 46:r:203:GLU:OE2  | 46:r:265:LYS:NZ   | 2.37                     | 0.51              |
| 47:s:231:ARG:HA   | 47:s:291:LEU:HD21 | 1.92                     | 0.51              |
| 9:A:1424:G:H2'    | 9:A:1425:G:H8     | 1.75                     | 0.51              |
| 30:Y:48:GLN:HA    | 30:Y:51:LEU:HD12  | 1.92                     | 0.51              |
| 9:A:29:G:H5'      | 13:E:124:LYS:HD2  | 1.93                     | 0.51              |
| 9:A:307:G:N2      | 26:R:44:HIS:HB3   | 2.26                     | 0.51              |
| 10:B:35:ARG:NH2   | 10:B:51:ILE:CA    | 2.65                     | 0.51              |
| 20:L:206:SER:OG   | 20:L:207:ALA:N    | 2.42                     | 0.51              |
| 25:Q:74:CYS:SG    | 25:Q:75:VAL:N     | 2.84                     | 0.51              |
| 50:v:349:GLN:OE1  | 50:v:393:MET:N    | 2.35                     | 0.51              |
| 53:y:339:ALA:HA   | 53:y:342:LYS:HD2  | 1.92                     | 0.51              |
| 9:A:1010:G:H2'    | 9:A:1011:A:H8     | 1.76                     | 0.51              |
| 9:A:1854:U:H2'    | 9:A:1855:G:C8     | 2.45                     | 0.51              |
| 17:I:63:VAL:HG11  | 17:I:71:ILE:HG13  | 1.92                     | 0.51              |
| 27:S:78:SER:HB3   | 27:S:92:ARG:HG2   | 1.91                     | 0.51              |
| 27:S:159:ARG:NH2  | 27:S:171:THR:O    | 2.43                     | 0.51              |
| 29:V:35:LEU:HD22  | 29:V:147:VAL:HG23 | 1.92                     | 0.51              |
| 33:b:60:LEU:HD11  | 33:b:89:MET:HE3   | 1.92                     | 0.51              |
| 36:e:63:PRO:HG2   | 36:e:96:LEU:HD23  | 1.93                     | 0.51              |
| 39:i:21:CYS:CB    | 39:i:26:ASN:H     | 2.23                     | 0.51              |
| 9:A:153:G:N3      | 27:S:13:GLN:NE2   | 2.38                     | 0.51              |
| 9:A:448:A:C5'     | 26:R:25:ARG:HA    | 2.35                     | 0.51              |
| 9:A:1285:G:H5'    | 41:m:35:ILE:HG22  | 1.92                     | 0.51              |
| 9:A:1593:C:P      | 36:e:103:HIS:HE2  | 2.33                     | 0.51              |
| 21:M:79:GLU:CA    | 21:M:82:ASP:HB2   | 2.34                     | 0.51              |
| 29:V:49:LEU:CD1   | 30:Y:47:LEU:HA    | 2.41                     | 0.51              |
| 43:o:241:ILE:HD13 | 43:o:314:TRP:HA   | 1.92                     | 0.51              |
| 53:y:422:GLU:HB3  | 53:y:433:ASN:HD21 | 1.76                     | 0.51              |
| 53:y:511:TYR:OH   | 53:y:611:ARG:NH1  | 2.44                     | 0.51              |
| 9:A:202:G:H5'     | 26:R:143:LYS:HE2  | 1.91                     | 0.51              |
| 9:A:642:U:P       | 12:D:39:ASN:HB2   | 2.51                     | 0.51              |
| 9:A:1863:A:N3     | 25:Q:79:ILE:HD11  | 2.26                     | 0.51              |
| 10:B:55:TYR:CZ    | 10:B:116:CYS:HB3  | 2.45                     | 0.51              |
| 27:S:12:CYS:SG    | 27:S:13:GLN:N     | 2.83                     | 0.51              |
| 44:p:54:TYR:HD2   | 53:y:272:LYS:CB   | 2.23                     | 0.51              |
| 9:A:202:G:H5'     | 26:R:143:LYS:CE   | 2.40                     | 0.51              |
| 31:Z:93:THR:HG21  | 31:Z:96:LEU:HD12  | 1.93                     | 0.51              |
| 40:k:140:TYR:CD1  | 40:k:140:TYR:C    | 2.89                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 49:u:544:GLN:O    | 49:u:548:GLU:N    | 2.40                     | 0.51              |
| 53:y:589:MET:O    | 53:y:595:GLN:NE2  | 2.43                     | 0.51              |
| 53:y:722:GLU:OE1  | 53:y:742:LYS:NZ   | 2.42                     | 0.51              |
| 9:A:10:G:H2'      | 9:A:11:A:H8       | 1.75                     | 0.51              |
| 9:A:868:G:O2'     | 15:G:115:LYS:HG3  | 2.11                     | 0.51              |
| 9:A:980:A:H2'     | 9:A:981:A:C8      | 2.46                     | 0.51              |
| 9:A:1010:G:H2'    | 9:A:1011:A:C8     | 2.45                     | 0.51              |
| 9:A:1413:G:H2'    | 9:A:1414:A:C8     | 2.46                     | 0.51              |
| 12:D:54:ARG:NH1   | 20:L:202:THR:HG22 | 2.22                     | 0.51              |
| 20:L:199:PRO:HG2  | 20:L:202:THR:HG21 | 1.93                     | 0.51              |
| 34:c:236:ILE:HG12 | 34:c:252:THR:HG22 | 1.92                     | 0.51              |
| 46:r:104:LYS:O    | 46:r:107:THR:OG1  | 2.25                     | 0.51              |
| 47:s:289:THR:HB   | 47:s:300:LEU:HD11 | 1.93                     | 0.51              |
| 52:x:25:PHE:O     | 52:x:26:ARG:NE    | 2.44                     | 0.51              |
| 53:y:602:ASP:OD1  | 53:y:602:ASP:N    | 2.40                     | 0.51              |
| 1:1:546:ILE:O     | 1:1:557:ASP:N     | 2.36                     | 0.51              |
| 23:O:182:LYS:O    | 23:O:186:ASN:ND2  | 2.43                     | 0.51              |
| 45:q:86:ASP:C     | 45:q:88:LYS:H     | 2.18                     | 0.51              |
| 46:r:14:PRO:HG3   | 46:r:36:LEU:HD21  | 1.91                     | 0.51              |
| 9:A:326:C:O2      | 9:A:328:U:N3      | 2.39                     | 0.50              |
| 16:H:45:THR:HG21  | 17:I:25:TRP:CZ3   | 2.46                     | 0.50              |
| 24:P:148:GLY:HA3  | 25:Q:28:ARG:HA    | 1.93                     | 0.50              |
| 49:u:564:GLU:O    | 49:u:568:ILE:N    | 2.42                     | 0.50              |
| 9:A:15:U:OP2      | 20:L:229:CYS:HB2  | 2.11                     | 0.50              |
| 9:A:45:A:N1       | 9:A:480:G:O2'     | 2.43                     | 0.50              |
| 9:A:56:G:OP2      | 28:T:115:LYS:NZ   | 2.32                     | 0.50              |
| 9:A:688:U:C6      | 15:G:122:LEU:CB   | 2.91                     | 0.50              |
| 9:A:1605:G:N1     | 9:A:1633:A:OP2    | 2.39                     | 0.50              |
| 15:G:149:ASP:OD1  | 15:G:149:ASP:N    | 2.43                     | 0.50              |
| 9:A:1082:A:HO2'   | 9:A:1842:C:HO2'   | 1.54                     | 0.50              |
| 11:C:137:PRO:HB2  | 11:C:150:PRO:HD2  | 1.92                     | 0.50              |
| 20:L:266:TYR:O    | 22:N:120:ARG:NH1  | 2.45                     | 0.50              |
| 21:M:116:ASN:OD1  | 21:M:116:ASN:N    | 2.45                     | 0.50              |
| 27:S:3:LEU:HB3    | 27:S:5:ILE:HD11   | 1.93                     | 0.50              |
| 9:A:921:G:H5'     | 16:H:21:LYS:HZ3   | 1.76                     | 0.50              |
| 9:A:1598:G:O5'    | 36:e:80:ARG:HD3   | 2.11                     | 0.50              |
| 9:A:1813:A:H3'    | 9:A:1814:G:H8     | 1.76                     | 0.50              |
| 15:G:99:ARG:HB3   | 15:G:120:ARG:HD3  | 1.94                     | 0.50              |
| 31:Z:219:PRO:HG2  | 34:c:189:ILE:O    | 2.11                     | 0.50              |
| 41:m:45:ARG:HG2   | 41:m:72:HIS:CD2   | 2.47                     | 0.50              |
| 47:s:182:ARG:O    | 47:s:186:ILE:N    | 2.44                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 49:u:80:GLN:HA    | 49:u:83:ILE:HB    | 1.94                     | 0.50              |
| 53:y:449:GLU:OE2  | 53:y:501:ARG:NH1  | 2.43                     | 0.50              |
| 5:6:286:ALA:HB2   | 5:6:320:MET:SD    | 2.52                     | 0.50              |
| 5:6:310:ALA:HB2   | 49:u:401:LEU:HD13 | 1.94                     | 0.50              |
| 9:A:154:U:O2      | 27:S:4:ASN:ND2    | 2.37                     | 0.50              |
| 9:A:1734:G:O2'    | 9:A:1800:A:N6     | 2.44                     | 0.50              |
| 11:C:45:ILE:HA    | 11:C:61:VAL:HG11  | 1.93                     | 0.50              |
| 23:O:52:THR:HG22  | 23:O:58:ALA:H     | 1.77                     | 0.50              |
| 23:O:62:LEU:O     | 23:O:88:THR:OG1   | 2.26                     | 0.50              |
| 34:c:155:ARG:O    | 34:c:166:VAL:N    | 2.43                     | 0.50              |
| 44:p:54:TYR:CZ    | 44:p:59:LEU:HB3   | 2.47                     | 0.50              |
| 47:s:251:ASP:OD2  | 51:w:26:C:O3'     | 2.30                     | 0.50              |
| 53:y:694:GLU:OE2  | 53:y:715:HIS:NE2  | 2.45                     | 0.50              |
| 1:1:380:ASP:N     | 1:1:389:VAL:O     | 2.43                     | 0.50              |
| 9:A:1113:A:O2'    | 9:A:1114:U:O4'    | 2.30                     | 0.50              |
| 9:A:1219:C:H2'    | 9:A:1220:A:H8     | 1.77                     | 0.50              |
| 9:A:1378:A:C6     | 22:N:136:GLU:OE2  | 2.65                     | 0.50              |
| 9:A:1550:G:O2'    | 9:A:1558:C:O2     | 2.28                     | 0.50              |
| 9:A:1599:U:OP2    | 36:e:46:ASN:ND2   | 2.44                     | 0.50              |
| 20:L:267:GLN:CG   | 22:N:120:ARG:HH22 | 2.24                     | 0.50              |
| 33:b:23:ASP:HA    | 33:b:26:LEU:HD12  | 1.94                     | 0.50              |
| 36:e:98:LYS:O     | 36:e:110:THR:N    | 2.45                     | 0.50              |
| 47:s:299:PHE:HE2  | 47:s:308:ARG:HB3  | 1.77                     | 0.50              |
| 9:A:584:A:P       | 12:D:169:ARG:HH22 | 2.35                     | 0.50              |
| 9:A:877:C:H2'     | 9:A:878:G:C8      | 2.47                     | 0.50              |
| 9:A:1464:C:H4'    | 21:M:60:ARG:NH2   | 2.26                     | 0.50              |
| 11:C:73:ASP:HB3   | 11:C:145:ARG:HH21 | 1.77                     | 0.50              |
| 17:I:142:GLU:HB3  | 17:I:145:THR:HG22 | 1.93                     | 0.50              |
| 26:R:103:LEU:HD22 | 26:R:170:LYS:HB3  | 1.94                     | 0.50              |
| 32:a:16:PHE:HE1   | 32:a:76:ILE:HG23  | 1.77                     | 0.50              |
| 50:v:208:LEU:HG   | 50:v:242:TYR:HD1  | 1.76                     | 0.50              |
| 9:A:10:G:H2'      | 9:A:11:A:C8       | 2.47                     | 0.50              |
| 9:A:483:C:H5''    | 13:E:48:LYS:HG3   | 1.94                     | 0.50              |
| 9:A:581:U:H5''    | 28:T:66:GLY:CA    | 2.42                     | 0.50              |
| 9:A:981:A:H2'     | 9:A:982:G:C8      | 2.46                     | 0.50              |
| 13:E:128:VAL:HG13 | 13:E:138:LYS:HE3  | 1.94                     | 0.50              |
| 16:H:3:LEU:HG     | 19:K:64:GLU:OE1   | 2.12                     | 0.50              |
| 19:K:40:ASP:OD1   | 19:K:40:ASP:N     | 2.42                     | 0.50              |
| 41:m:93:LYS:H     | 41:m:104:VAL:H    | 1.60                     | 0.50              |
| 46:r:71:VAL:HG21  | 46:r:85:LEU:HD13  | 1.94                     | 0.50              |
| 47:s:296:ARG:NH2  | 51:w:69:G:P       | 2.85                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 49:u:476:ARG:HB2  | 53:y:795:TYR:HE1  | 1.76                     | 0.50              |
| 52:x:44:ASP:OD2   | 53:y:645:LEU:HD11 | 2.12                     | 0.50              |
| 53:y:330:ILE:O    | 53:y:334:ASN:ND2  | 2.44                     | 0.50              |
| 2:3:8:ARG:O       | 2:3:12:GLY:N      | 2.39                     | 0.50              |
| 5:6:317:ARG:NH1   | 49:u:399:ASN:OD1  | 2.39                     | 0.50              |
| 9:A:1048:G:OP1    | 24:P:144:GLY:N    | 2.45                     | 0.50              |
| 9:A:1055:A:N6     | 9:A:1061:U:OP2    | 2.45                     | 0.50              |
| 10:B:40:ILE:HD11  | 10:B:44:PHE:HB2   | 1.94                     | 0.50              |
| 24:P:117:ARG:NH2  | 25:Q:48:ALA:O     | 2.45                     | 0.50              |
| 29:V:124:ASP:HB2  | 29:V:141:VAL:HG22 | 1.94                     | 0.50              |
| 49:u:561:SER:HA   | 49:u:564:GLU:HB2  | 1.94                     | 0.50              |
| 9:A:1445:U:H4'    | 38:h:57:PRO:HG3   | 1.94                     | 0.49              |
| 9:A:1531:A:H4'    | 9:A:1605:G:H4'    | 1.94                     | 0.49              |
| 20:L:254:ASP:N    | 20:L:254:ASP:OD1  | 2.43                     | 0.49              |
| 39:i:8:TRP:HE1    | 39:i:12:ARG:HB2   | 1.76                     | 0.49              |
| 43:o:243:VAL:HB   | 43:o:283:ALA:HB3  | 1.93                     | 0.49              |
| 9:A:677:G:N1      | 9:A:1027:A:OP2    | 2.30                     | 0.49              |
| 11:C:171:ASP:HB3  | 11:C:235:TRP:CZ3  | 2.47                     | 0.49              |
| 19:K:43:THR:OG1   | 19:K:45:ARG:NH2   | 2.38                     | 0.49              |
| 53:y:833:ALA:HB2  | 53:y:844:MET:HE3  | 1.93                     | 0.49              |
| 2:3:112:CYS:CB    | 4:5:498:LYS:CB    | 2.90                     | 0.49              |
| 9:A:648:A:H4'     | 13:E:104:GLY:O    | 2.11                     | 0.49              |
| 9:A:1060:A:O2'    | 9:A:1062:A:N7     | 2.38                     | 0.49              |
| 9:A:1454:A:H3'    | 21:M:5:ARG:HH11   | 1.77                     | 0.49              |
| 16:H:15:GLU:O     | 16:H:23:ARG:NE    | 2.38                     | 0.49              |
| 25:Q:95:ARG:O     | 25:Q:96:THR:C     | 2.54                     | 0.49              |
| 29:V:47:LYS:HA    | 30:Y:115:TYR:OH   | 2.11                     | 0.49              |
| 29:V:126:THR:HG21 | 42:n:27:CYS:SG    | 2.52                     | 0.49              |
| 30:Y:11:GLN:HA    | 30:Y:24:HIS:HA    | 1.94                     | 0.49              |
| 30:Y:93:VAL:HA    | 30:Y:108:ILE:HD11 | 1.93                     | 0.49              |
| 44:p:54:TYR:CD1   | 53:y:269:ALA:HB1  | 2.48                     | 0.49              |
| 49:u:387:VAL:HG12 | 49:u:410:VAL:HB   | 1.93                     | 0.49              |
| 49:u:520:ARG:HA   | 49:u:523:LEU:HD12 | 1.94                     | 0.49              |
| 9:A:77:A:C2       | 27:S:175:LYS:HG3  | 2.39                     | 0.49              |
| 9:A:110:U:H5''    | 11:C:205:PHE:CE1  | 2.48                     | 0.49              |
| 9:A:170:A:OP1     | 27:S:136:LYS:N    | 2.30                     | 0.49              |
| 9:A:1086:G:H4'    | 25:Q:8:ASN:HD21   | 1.78                     | 0.49              |
| 9:A:1092:G:H2'    | 9:A:1093:A:H8     | 1.77                     | 0.49              |
| 9:A:1105:G:O3'    | 16:H:69:GLY:HA3   | 2.12                     | 0.49              |
| 9:A:1308:U:H4'    | 40:k:133:ALA:CA   | 2.42                     | 0.49              |
| 9:A:1611:G:OP1    | 37:f:121:ARG:NH2  | 2.45                     | 0.49              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 9:A:1758:G:H21   | 9:A:1775:U:H3     | 1.60                     | 0.49              |
| 10:B:109:MET:HE1 | 10:B:140:PHE:CE1  | 2.46                     | 0.49              |
| 11:C:181:CYS:SG  | 11:C:225:ILE:HG23 | 2.52                     | 0.49              |
| 15:G:17:ASP:O    | 15:G:21:SER:N     | 2.45                     | 0.49              |
| 23:O:128:LYS:CE  | 53:y:307:GLY:O    | 2.60                     | 0.49              |
| 16:H:8:LEU:CD2   | 18:J:62:VAL:HG11  | 2.42                     | 0.49              |
| 20:L:70:VAL:HG11 | 20:L:93:ILE:HG23  | 1.93                     | 0.49              |
| 23:O:48:LEU:HD21 | 24:P:53:ILE:CD1   | 2.42                     | 0.49              |
| 24:P:146:ARG:C   | 24:P:148:GLY:H    | 2.20                     | 0.49              |
| 53:y:121:TRP:HZ2 | 53:y:139:SER:HA   | 1.77                     | 0.49              |
| 9:A:678:U:OP1    | 17:I:127:ARG:NH2  | 2.45                     | 0.49              |
| 9:A:1380:C:OP1   | 22:N:102:ARG:NH1  | 2.46                     | 0.49              |
| 9:A:1674:G:H5''  | 29:V:86:LYS:CD    | 2.42                     | 0.49              |
| 30:Y:81:ILE:HG13 | 30:Y:82:TYR:N     | 2.27                     | 0.49              |
| 41:m:91:LEU:HB2  | 41:m:104:VAL:HB   | 1.95                     | 0.49              |
| 52:x:225:HIS:O   | 52:x:374:ARG:NH2  | 2.44                     | 0.49              |
| 53:y:601:ALA:O   | 53:y:606:GLN:NE2  | 2.46                     | 0.49              |
| 9:A:688:U:N1     | 15:G:122:LEU:HD13 | 2.28                     | 0.49              |
| 9:A:1268:C:H4'   | 33:b:100:LYS:HG3  | 1.94                     | 0.49              |
| 10:B:109:MET:CE  | 10:B:140:PHE:CD1  | 2.96                     | 0.49              |
| 15:G:47:ALA:HB3  | 15:G:63:PHE:HD2   | 1.78                     | 0.49              |
| 21:M:12:ALA:HB1  | 31:Z:208:VAL:HG11 | 1.94                     | 0.49              |
| 29:V:52:SER:HA   | 30:Y:82:TYR:OH    | 2.12                     | 0.49              |
| 46:r:183:ARG:NH1 | 51:w:53:A:C4      | 2.80                     | 0.49              |
| 9:A:873:G:H22    | 10:B:152:LYS:HB2  | 1.77                     | 0.49              |
| 9:A:1313:A:H5''  | 32:a:5:LYS:HD3    | 1.95                     | 0.49              |
| 9:A:1565:C:C5    | 35:d:101:ARG:CZ   | 2.96                     | 0.49              |
| 21:M:78:ARG:HD3  | 22:N:89:LYS:NZ    | 2.27                     | 0.49              |
| 23:O:59:SER:OG   | 23:O:63:LYS:NZ    | 2.38                     | 0.49              |
| 29:V:125:SER:HA  | 29:V:138:ALA:HA   | 1.95                     | 0.49              |
| 32:a:58:VAL:HG12 | 32:a:71:LEU:HA    | 1.94                     | 0.49              |
| 33:b:73:PRO:HG2  | 33:b:92:SER:HA    | 1.93                     | 0.49              |
| 43:o:250:THR:O   | 43:o:251:ARG:NH1  | 2.43                     | 0.49              |
| 44:p:67:PHE:HZ   | 44:p:96:PHE:HB2   | 1.78                     | 0.49              |
| 50:v:205:LEU:HB2 | 52:x:23:GLU:HG2   | 1.94                     | 0.49              |
| 51:w:14:A:O2'    | 51:w:16:C:N4      | 2.46                     | 0.49              |
| 9:A:1648:G:H3'   | 30:Y:126:ARG:O    | 2.11                     | 0.49              |
| 33:b:28:MET:HB2  | 33:b:32:GLN:HB2   | 1.94                     | 0.49              |
| 40:k:126:CYS:CB  | 40:k:130:VAL:HG21 | 2.43                     | 0.49              |
| 43:o:296:ALA:O   | 43:o:300:VAL:HG12 | 2.12                     | 0.49              |
| 9:A:92:A:O3'     | 11:C:3:ARG:HB2    | 2.13                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:A:1220:A:H2'    | 9:A:1221:G:O4'    | 2.13                     | 0.49              |
| 9:A:1565:C:H5     | 35:d:101:ARG:CZ   | 2.26                     | 0.49              |
| 9:A:1630:A:OP1    | 37:f:37:GLY:CA    | 2.61                     | 0.49              |
| 9:A:1741:U:OP1    | 26:R:42:ARG:NH1   | 2.42                     | 0.49              |
| 9:A:1854:U:H2'    | 9:A:1855:G:H8     | 1.78                     | 0.49              |
| 13:E:124:LYS:HG2  | 13:E:129:SER:HA   | 1.94                     | 0.49              |
| 21:M:19:LYS:HE3   | 31:Z:213:PRO:HD3  | 1.95                     | 0.49              |
| 29:V:103:LEU:HD21 | 36:e:67:LEU:HB3   | 1.95                     | 0.49              |
| 31:Z:45:ARG:HH11  | 31:Z:85:GLU:HG3   | 1.78                     | 0.49              |
| 33:b:81:ARG:NH2   | 33:b:117:GLY:O    | 2.46                     | 0.49              |
| 44:p:54:TYR:CE1   | 44:p:102:LEU:HD11 | 2.47                     | 0.49              |
| 44:p:99:GLU:HG2   | 44:p:100:ILE:HG13 | 1.93                     | 0.49              |
| 47:s:183:VAL:HA   | 47:s:186:ILE:HG13 | 1.95                     | 0.49              |
| 47:s:188:ARG:NH1  | 47:s:194:MET:HA   | 2.24                     | 0.49              |
| 5:6:204:ALA:O     | 5:6:208:ILE:N     | 2.46                     | 0.48              |
| 5:6:293:SER:HA    | 5:6:328:THR:O     | 2.13                     | 0.48              |
| 9:A:750:C:H41     | 9:A:793:G:H1'     | 1.78                     | 0.48              |
| 9:A:931:C:OP2     | 23:O:159:GLN:HG3  | 2.13                     | 0.48              |
| 9:A:1422:G:O2'    | 9:A:1424:G:OP2    | 2.30                     | 0.48              |
| 10:B:47:PRO:HD3   | 10:B:62:PHE:CD1   | 2.47                     | 0.48              |
| 24:P:34:PHE:HE1   | 24:P:100:THR:HA   | 1.78                     | 0.48              |
| 34:c:32:LEU:HB2   | 34:c:71:ILE:HD11  | 1.95                     | 0.48              |
| 47:s:195:VAL:HG13 | 48:t:193:ASP:O    | 2.13                     | 0.48              |
| 52:x:360:TYR:HE1  | 52:x:374:ARG:HG3  | 1.78                     | 0.48              |
| 8:9:5:TRP:HB3     | 9:A:1852:C:H5     | 1.77                     | 0.48              |
| 9:A:370:G:H4'     | 9:A:371:A:O5'     | 2.13                     | 0.48              |
| 9:A:483:C:C5'     | 13:E:48:LYS:HG3   | 2.43                     | 0.48              |
| 9:A:1594:A:H1'    | 35:d:16:ARG:NH2   | 2.28                     | 0.48              |
| 9:A:1679:A:H2'    | 29:V:60:ARG:CD    | 2.37                     | 0.48              |
| 9:A:502:C:O4'     | 11:C:66:MET:HG3   | 2.14                     | 0.48              |
| 9:A:855:G:H4'     | 10:B:71:ARG:HH12  | 1.77                     | 0.48              |
| 21:M:98:VAL:HG13  | 21:M:102:THR:HG23 | 1.95                     | 0.48              |
| 26:R:66:SER:HA    | 26:R:73:THR:HA    | 1.95                     | 0.48              |
| 27:S:134:GLY:HA3  | 27:S:158:VAL:HG11 | 1.95                     | 0.48              |
| 37:f:26:ILE:HD13  | 37:f:56:ALA:HA    | 1.95                     | 0.48              |
| 43:o:246:LEU:HD22 | 43:o:250:THR:HG21 | 1.94                     | 0.48              |
| 51:w:15:G:H1'     | 51:w:21:G:H1'     | 1.95                     | 0.48              |
| 52:x:432:LEU:HD12 | 52:x:476:PHE:HZ   | 1.77                     | 0.48              |
| 53:y:78:LYS:HA    | 53:y:81:GLU:HG2   | 1.95                     | 0.48              |
| 9:A:989:C:OP2     | 23:O:117:TRP:N    | 2.47                     | 0.48              |
| 9:A:1004:U:P      | 23:O:165:ARG:NH2  | 2.84                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 31:Z:225:GLU:OE2  | 31:Z:227:LYS:NZ   | 2.43                     | 0.48              |
| 34:c:256:ILE:HD13 | 34:c:289:LEU:HD21 | 1.95                     | 0.48              |
| 46:r:104:LYS:HD3  | 46:r:150:TYR:HB2  | 1.95                     | 0.48              |
| 9:A:545:A:O2'     | 9:A:546:G:O4'     | 2.24                     | 0.48              |
| 9:A:747:U:H2'     | 9:A:748:C:C2      | 2.49                     | 0.48              |
| 9:A:1631:U:H4'    | 37:f:34:LYS:CE    | 2.42                     | 0.48              |
| 19:K:23:ILE:HG21  | 20:L:249:SER:HA   | 1.94                     | 0.48              |
| 20:L:87:PRO:HG3   | 22:N:140:VAL:HA   | 1.96                     | 0.48              |
| 31:Z:96:LEU:HD13  | 31:Z:198:ILE:HG23 | 1.94                     | 0.48              |
| 32:a:67:PHE:HB3   | 32:a:69:TRP:CZ2   | 2.47                     | 0.48              |
| 45:q:86:ASP:O     | 45:q:88:LYS:N     | 2.46                     | 0.48              |
| 49:u:319:SER:HA   | 49:u:322:VAL:HG12 | 1.94                     | 0.48              |
| 9:A:1121:G:O2'    | 23:O:204:ILE:O    | 2.24                     | 0.48              |
| 9:A:1853:C:H2'    | 9:A:1854:U:C6     | 2.49                     | 0.48              |
| 15:G:105:THR:HG23 | 15:G:107:LYS:H    | 1.78                     | 0.48              |
| 39:i:24:CYS:SG    | 39:i:26:ASN:HB2   | 2.54                     | 0.48              |
| 9:A:323:C:O2'     | 9:A:328:U:O4      | 2.30                     | 0.48              |
| 9:A:1000:C:N4     | 25:Q:15:ARG:HB3   | 2.29                     | 0.48              |
| 16:H:20:LYS:HG3   | 16:H:21:LYS:HG2   | 1.95                     | 0.48              |
| 21:M:29:HIS:HB3   | 34:c:83:TRP:CZ3   | 2.49                     | 0.48              |
| 24:P:113:GLN:HB2  | 25:Q:46:GLU:OE2   | 2.13                     | 0.48              |
| 31:Z:28:GLU:HG2   | 31:Z:69:LEU:HD21  | 1.96                     | 0.48              |
| 39:i:22:ARG:HE    | 39:i:37:ASN:HB2   | 1.78                     | 0.48              |
| 46:r:22:VAL:HG23  | 46:r:36:LEU:HA    | 1.94                     | 0.48              |
| 9:A:798:G:C6      | 15:G:107:LYS:C    | 2.92                     | 0.48              |
| 9:A:1740:C:H5''   | 26:R:58:LEU:HD11  | 1.94                     | 0.48              |
| 46:r:183:ARG:CZ   | 51:w:53:A:N3      | 2.77                     | 0.48              |
| 52:x:301:ASP:HB3  | 52:x:309:PRO:HD3  | 1.94                     | 0.48              |
| 9:A:1617:G:N1     | 9:A:1620:A:OP2    | 2.46                     | 0.48              |
| 11:C:114:ILE:HD12 | 11:C:118:GLU:HG2  | 1.96                     | 0.48              |
| 14:F:105:ARG:O    | 14:F:109:ARG:N    | 2.45                     | 0.48              |
| 21:M:99:ASP:HB2   | 21:M:102:THR:HG22 | 1.95                     | 0.48              |
| 29:V:49:LEU:HD12  | 30:Y:50:LYS:H     | 1.79                     | 0.48              |
| 34:c:245:ARG:NH1  | 34:c:295:GLY:O    | 2.47                     | 0.48              |
| 43:o:300:VAL:HG13 | 43:o:312:VAL:HG21 | 1.96                     | 0.48              |
| 50:v:261:VAL:HG23 | 50:v:262:ILE:HG13 | 1.96                     | 0.48              |
| 52:x:322:ASN:OD1  | 52:x:323:PHE:N    | 2.47                     | 0.48              |
| 9:A:583:A:H2'     | 9:A:584:A:C8      | 2.49                     | 0.48              |
| 9:A:1207:G:N2     | 9:A:1837:G:H2'    | 2.28                     | 0.48              |
| 9:A:1567:G:H5'    | 35:d:33:TRP:CE2   | 2.49                     | 0.48              |
| 9:A:1649:U:OP1    | 30:Y:128:GLU:N    | 2.46                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:M:34:VAL:HG22  | 34:c:150:TRP:CH2  | 2.49                     | 0.48              |
| 24:P:118:ALA:C    | 24:P:120:ALA:H    | 2.21                     | 0.48              |
| 49:u:52:LEU:HD12  | 49:u:89:VAL:HG23  | 1.95                     | 0.48              |
| 9:A:572:U:OP2     | 28:T:37:LYS:NZ    | 2.39                     | 0.47              |
| 9:A:1005:G:OP2    | 23:O:162:ARG:NH1  | 2.47                     | 0.47              |
| 9:A:1125:C:H5'    | 21:M:126:MET:O    | 2.14                     | 0.47              |
| 9:A:1229:G:H4'    | 9:A:1633:A:H2     | 1.79                     | 0.47              |
| 9:A:1304:U:H5'    | 40:k:95:ARG:N     | 2.29                     | 0.47              |
| 14:F:80:LEU:HB3   | 45:q:82:ARG:HH12  | 1.78                     | 0.47              |
| 20:L:172:ASN:OD1  | 20:L:172:ASN:N    | 2.47                     | 0.47              |
| 21:M:39:ALA:HA    | 31:Z:211:VAL:HG23 | 1.96                     | 0.47              |
| 21:M:77:GLU:C     | 21:M:79:GLU:N     | 2.67                     | 0.47              |
| 40:k:141:CYS:O    | 40:k:144:CYS:HB2  | 2.14                     | 0.47              |
| 45:q:61:ILE:HD12  | 45:q:91:VAL:HG21  | 1.96                     | 0.47              |
| 9:A:873:G:H22     | 10:B:152:LYS:CB   | 2.27                     | 0.47              |
| 9:A:1275:G:O2'    | 9:A:1321:G:N2     | 2.39                     | 0.47              |
| 9:A:1752:C:H6     | 9:A:1779:G:H1     | 1.61                     | 0.47              |
| 9:A:1754:G:H2'    | 9:A:1755:C:H4'    | 1.95                     | 0.47              |
| 20:L:144:SER:HB3  | 20:L:150:ALA:HB2  | 1.96                     | 0.47              |
| 24:P:148:GLY:CA   | 25:Q:28:ARG:HA    | 2.44                     | 0.47              |
| 36:e:50:PHE:HB2   | 37:f:4:VAL:HG12   | 1.96                     | 0.47              |
| 9:A:70:G:N2       | 9:A:80:G:O6       | 2.47                     | 0.47              |
| 9:A:1551:U:OP1    | 31:Z:9:ARG:NH2    | 2.46                     | 0.47              |
| 23:O:190:PRO:HB2  | 49:u:18:PHE:CE1   | 2.50                     | 0.47              |
| 24:P:125:LYS:HB3  | 25:Q:58:VAL:HG13  | 1.96                     | 0.47              |
| 28:T:29:HIS:NE2   | 28:T:69:THR:OG1   | 2.46                     | 0.47              |
| 30:Y:58:LEU:HB2   | 30:Y:63:PHE:HE1   | 1.79                     | 0.47              |
| 32:a:23:ALA:HB3   | 32:a:69:TRP:CH2   | 2.48                     | 0.47              |
| 46:r:16:VAL:HG22  | 46:r:17:GLU:HG2   | 1.95                     | 0.47              |
| 47:s:195:VAL:CG1  | 48:t:193:ASP:O    | 2.62                     | 0.47              |
| 53:y:515:ASP:H    | 53:y:579:HIS:CE1  | 2.31                     | 0.47              |
| 5:6:289:ASN:HA    | 5:6:332:VAL:HG22  | 1.97                     | 0.47              |
| 28:T:5:VAL:O      | 28:T:43:LYS:NZ    | 2.46                     | 0.47              |
| 31:Z:195:THR:HA   | 31:Z:201:LYS:HE2  | 1.95                     | 0.47              |
| 49:u:144:LEU:HD22 | 53:y:467:GLN:HB3  | 1.95                     | 0.47              |
| 1:1:291:GLY:HA3   | 1:1:363:GLU:H     | 1.79                     | 0.47              |
| 9:A:1535:U:H5'    | 29:V:169:ILE:HG22 | 1.97                     | 0.47              |
| 9:A:1680:G:H4'    | 42:n:20:ARG:HD2   | 1.95                     | 0.47              |
| 19:K:41:LYS:HD3   | 22:N:5:LEU:HD11   | 1.96                     | 0.47              |
| 20:L:222:CYS:SG   | 20:L:223:TYR:N    | 2.87                     | 0.47              |
| 30:Y:34:VAL:HB    | 30:Y:42:ILE:HD11  | 1.95                     | 0.47              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:1:648:ILE:HA    | 1:1:688:GLY:O    | 2.15                     | 0.47              |
| 9:A:53:C:O2'      | 9:A:507:G:N7     | 2.40                     | 0.47              |
| 9:A:1233:G:N3     | 9:A:1252:C:O2'   | 2.40                     | 0.47              |
| 9:A:1337:C:H2'    | 9:A:1338:G:H8    | 1.79                     | 0.47              |
| 9:A:1712:A:H2'    | 9:A:1713:C:C6    | 2.50                     | 0.47              |
| 30:Y:11:GLN:HB3   | 30:Y:24:HIS:HB2  | 1.96                     | 0.47              |
| 30:Y:81:ILE:HA    | 30:Y:84:ILE:HD12 | 1.97                     | 0.47              |
| 43:o:242:ARG:N    | 43:o:313:GLU:O   | 2.46                     | 0.47              |
| 44:p:48:GLN:HA    | 44:p:82:VAL:HG12 | 1.96                     | 0.47              |
| 50:v:284:GLU:OE1  | 53:y:586:ARG:NH1 | 2.48                     | 0.47              |
| 52:x:43:ALA:HB2   | 53:y:609:TYR:HD2 | 1.79                     | 0.47              |
| 3:4:209:GLY:HA3   | 5:6:113:MET:CB   | 2.45                     | 0.47              |
| 9:A:24:C:OP1      | 12:D:11:LYS:HE3  | 2.13                     | 0.47              |
| 9:A:533:A:H2'     | 9:A:534:G:C8     | 2.49                     | 0.47              |
| 9:A:1281:G:H2'    | 9:A:1282:A:H8    | 1.79                     | 0.47              |
| 9:A:1578:U:O3'    | 31:Z:6:SER:HA    | 2.15                     | 0.47              |
| 21:M:23:ARG:NH1   | 34:c:149:GLU:OE2 | 2.47                     | 0.47              |
| 21:M:34:VAL:HG12  | 21:M:38:ILE:HD13 | 1.97                     | 0.47              |
| 29:V:30:ILE:HG21  | 29:V:36:GLN:HA   | 1.96                     | 0.47              |
| 34:c:183:LYS:HD3  | 34:c:183:LYS:HA  | 1.68                     | 0.47              |
| 35:d:104:LEU:HD13 | 35:d:121:ARG:HD2 | 1.95                     | 0.47              |
| 41:m:69:CYS:HA    | 41:m:74:ILE:HD12 | 1.95                     | 0.47              |
| 41:m:96:ARG:HG2   | 41:m:96:ARG:O    | 2.13                     | 0.47              |
| 46:r:209:LYS:O    | 46:r:213:ARG:N   | 2.44                     | 0.47              |
| 49:u:567:ARG:HE   | 49:u:572:ARG:HG3 | 1.79                     | 0.47              |
| 52:x:397:ASN:N    | 52:x:397:ASN:OD1 | 2.47                     | 0.47              |
| 1:1:378:LEU:N     | 1:1:391:PHE:O    | 2.43                     | 0.47              |
| 9:A:677:G:H5'     | 17:I:120:SER:OG  | 2.15                     | 0.47              |
| 9:A:1084:A:OP1    | 9:A:1858:G:O2'   | 2.30                     | 0.47              |
| 9:A:1113:A:H4'    | 23:O:202:GLN:HB3 | 1.97                     | 0.47              |
| 13:E:68:LYS:HB3   | 13:E:91:LEU:HD22 | 1.97                     | 0.47              |
| 15:G:43:LEU:HD22  | 15:G:72:PHE:HD1  | 1.79                     | 0.47              |
| 17:I:69:ASN:OD1   | 17:I:69:ASN:N    | 2.47                     | 0.47              |
| 21:M:82:ASP:O     | 21:M:85:VAL:HG22 | 2.15                     | 0.47              |
| 50:v:229:ARG:HD3  | 50:v:229:ARG:HA  | 1.66                     | 0.47              |
| 51:w:72:A:C8      | 51:w:73:C:H2'    | 2.49                     | 0.47              |
| 9:A:509:OMG:HM23  | 9:A:509:OMG:H1'  | 1.52                     | 0.47              |
| 9:A:1122:A:H4'    | 23:O:205:TYR:CD2 | 2.50                     | 0.47              |
| 9:A:1298:G:H1'    | 33:b:79:HIS:CG   | 2.50                     | 0.47              |
| 9:A:1643:U:H2'    | 9:A:1644:C:C6    | 2.50                     | 0.47              |
| 9:A:1754:G:OP1    | 9:A:1780:G:N1    | 2.48                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 12:D:107:GLU:O    | 12:D:113:GLN:NE2  | 2.40                     | 0.47              |
| 15:G:60:ILE:HB    | 15:G:92:VAL:HG23  | 1.95                     | 0.47              |
| 19:K:41:LYS:HD3   | 22:N:5:LEU:CD1    | 2.45                     | 0.47              |
| 22:N:183:LEU:O    | 22:N:187:GLY:N    | 2.48                     | 0.47              |
| 23:O:175:GLU:OE1  | 23:O:187:LYS:NZ   | 2.43                     | 0.47              |
| 30:Y:58:LEU:HB3   | 30:Y:62:ARG:HD2   | 1.97                     | 0.47              |
| 31:Z:20:GLU:HB2   | 32:a:64:TRP:CD2   | 2.50                     | 0.47              |
| 32:a:32:HIS:HB2   | 32:a:42:ASN:HA    | 1.97                     | 0.47              |
| 32:a:32:HIS:CE1   | 32:a:34:GLU:HB2   | 2.48                     | 0.47              |
| 33:b:111:MET:HA   | 37:f:117:ILE:HD11 | 1.97                     | 0.47              |
| 53:y:763:GLY:HA2  | 53:y:767:ASP:HB2  | 1.97                     | 0.47              |
| 7:8:245:LEU:N     | 49:u:522:GLN:OE1  | 2.37                     | 0.47              |
| 8:9:2:ARG:HD3     | 8:9:5:TRP:CD1     | 2.49                     | 0.47              |
| 9:A:476:A:N3      | 9:A:488:U:O2'     | 2.39                     | 0.47              |
| 9:A:962:A:H5''    | 24:P:66:ARG:HG3   | 1.97                     | 0.47              |
| 9:A:1856:C:OP1    | 24:P:141:ARG:NH1  | 2.44                     | 0.47              |
| 16:H:7:LEU:CD1    | 18:J:24:GLN:HB3   | 2.45                     | 0.47              |
| 21:M:17:ILE:HG13  | 21:M:18:GLU:N     | 2.30                     | 0.47              |
| 34:c:221:LEU:HD23 | 34:c:221:LEU:HA   | 1.79                     | 0.47              |
| 41:m:121:LYS:O    | 41:m:125:GLU:N    | 2.40                     | 0.47              |
| 49:u:23:LYS:HB3   | 49:u:26:PRO:HD2   | 1.97                     | 0.47              |
| 49:u:483:ARG:O    | 49:u:492:SER:N    | 2.44                     | 0.47              |
| 49:u:551:GLN:O    | 49:u:555:THR:N    | 2.41                     | 0.47              |
| 50:v:243:LEU:HB3  | 50:v:249:MET:SD   | 2.55                     | 0.47              |
| 53:y:50:ARG:HH21  | 53:y:55:LYS:HD2   | 1.79                     | 0.47              |
| 1:1:342:TRP:HA    | 1:1:349:LEU:HA    | 1.97                     | 0.46              |
| 3:4:288:GLN:CB    | 5:6:348:GLN:NE2   | 2.79                     | 0.46              |
| 9:A:562:U:OP2     | 12:D:171:GLY:HA3  | 2.15                     | 0.46              |
| 9:A:821:G:N1      | 12:D:150:ARG:HG3  | 2.30                     | 0.46              |
| 9:A:1336:C:OP2    | 31:Z:185:LYS:HE2  | 2.16                     | 0.46              |
| 9:A:1702:G:H2'    | 9:A:1703:OMC:C6   | 2.50                     | 0.46              |
| 29:V:140:ASP:HB2  | 42:n:46:VAL:CG1   | 2.39                     | 0.46              |
| 37:f:105:ASN:OD1  | 37:f:108:ARG:NH1  | 2.48                     | 0.46              |
| 44:p:54:TYR:CD2   | 53:y:272:LYS:CB   | 2.98                     | 0.46              |
| 45:q:61:ILE:CG2   | 45:q:66:ARG:HD3   | 2.45                     | 0.46              |
| 49:u:549:GLN:HA   | 49:u:552:LEU:HB3  | 1.97                     | 0.46              |
| 50:v:385:ASP:OD2  | 50:v:390:HIS:N    | 2.48                     | 0.46              |
| 1:1:357:ILE:O     | 1:1:371:PHE:N     | 2.45                     | 0.46              |
| 9:A:492:C:OP2     | 28:T:107:ARG:NH2  | 2.47                     | 0.46              |
| 9:A:616:A:H1'     | 14:F:86:VAL:HG23  | 1.96                     | 0.46              |
| 9:A:1102:G:P      | 23:O:151:ARG:HH11 | 2.39                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:A:1183:A:H2'    | 9:A:1184:G:H8     | 1.80                     | 0.46              |
| 9:A:1300:U:C2     | 33:b:51:ARG:HD3   | 2.50                     | 0.46              |
| 16:H:38:PRO:HD3   | 16:H:77:CYS:HA    | 1.96                     | 0.46              |
| 25:Q:13:LYS:H     | 25:Q:15:ARG:HE    | 1.63                     | 0.46              |
| 25:Q:38:LYS:HB3   | 25:Q:71:LEU:HB2   | 1.97                     | 0.46              |
| 26:R:119:LEU:HD21 | 26:R:153:LYS:HG2  | 1.98                     | 0.46              |
| 32:a:49:MET:HG3   | 32:a:69:TRP:CE3   | 2.50                     | 0.46              |
| 39:i:45:GLN:C     | 39:i:47:ALA:H     | 2.23                     | 0.46              |
| 43:o:270:LEU:HD11 | 43:o:279:SER:HB2  | 1.98                     | 0.46              |
| 44:p:104:LYS:HD3  | 44:p:104:LYS:HA   | 1.78                     | 0.46              |
| 49:u:179:GLN:NE2  | 49:u:231:GLU:OE1  | 2.47                     | 0.46              |
| 49:u:389:ASP:N    | 49:u:389:ASP:OD1  | 2.45                     | 0.46              |
| 53:y:643:LYS:HG3  | 53:y:650:LEU:HB2  | 1.96                     | 0.46              |
| 53:y:785:GLU:HG2  | 53:y:813:LEU:HD11 | 1.96                     | 0.46              |
| 9:A:54:A:H5'      | 28:T:108:LYS:HZ3  | 1.80                     | 0.46              |
| 9:A:584:A:H2'     | 9:A:585:C:C6      | 2.50                     | 0.46              |
| 9:A:1138:C:C6     | 19:K:61:ARG:HD3   | 2.50                     | 0.46              |
| 15:G:58:LYS:HE2   | 15:G:90:LYS:HE2   | 1.97                     | 0.46              |
| 18:J:94:LEU:O     | 20:L:183:LYS:NZ   | 2.29                     | 0.46              |
| 24:P:28:PHE:CZ    | 25:Q:58:VAL:HG21  | 2.42                     | 0.46              |
| 24:P:113:GLN:HB2  | 25:Q:46:GLU:CD    | 2.40                     | 0.46              |
| 32:a:47:LYS:HA    | 32:a:47:LYS:HD3   | 1.81                     | 0.46              |
| 49:u:571:ARG:HA   | 49:u:571:ARG:HD2  | 1.78                     | 0.46              |
| 50:v:93:LYS:O     | 50:v:97:ASP:N     | 2.48                     | 0.46              |
| 53:y:596:ASP:OD1  | 53:y:596:ASP:N    | 2.49                     | 0.46              |
| 17:I:47:PRO:HG2   | 17:I:72:LEU:HD12  | 1.97                     | 0.46              |
| 9:A:223:C:H2'     | 9:A:224:A:H8      | 1.80                     | 0.46              |
| 9:A:1102:G:OP1    | 23:O:151:ARG:NH1  | 2.49                     | 0.46              |
| 9:A:1674:G:C5'    | 29:V:86:LYS:HB2   | 2.46                     | 0.46              |
| 20:L:123:ARG:HD2  | 20:L:145:LYS:HE2  | 1.97                     | 0.46              |
| 20:L:270:THR:HG21 | 22:N:69:GLU:CB    | 2.46                     | 0.46              |
| 20:L:270:THR:HG21 | 22:N:69:GLU:HG3   | 1.98                     | 0.46              |
| 25:Q:73:TYR:HB3   | 25:Q:78:ALA:HB2   | 1.97                     | 0.46              |
| 27:S:57:ASP:OD1   | 27:S:58:LYS:N     | 2.48                     | 0.46              |
| 47:s:227:LYS:HB3  | 47:s:227:LYS:HE3  | 1.64                     | 0.46              |
| 9:A:1360:U:O2'    | 9:A:1379:A:OP2    | 2.25                     | 0.46              |
| 9:A:1398:G:H22    | 9:A:1448:A:H2     | 1.62                     | 0.46              |
| 9:A:1865:C:OP2    | 25:Q:92:ARG:HG2   | 2.16                     | 0.46              |
| 11:C:60:GLU:CD    | 28:T:20:ARG:HH12  | 2.23                     | 0.46              |
| 12:D:84:ILE:HG13  | 12:D:86:VAL:HG13  | 1.98                     | 0.46              |
| 21:M:91:LEU:O     | 22:N:20:ALA:HB1   | 2.16                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 43:o:303:PHE:HB3  | 43:o:310:LEU:HD21 | 1.98                     | 0.46              |
| 46:r:56:ILE:HD12  | 46:r:56:ILE:HA    | 1.84                     | 0.46              |
| 49:u:411:LEU:HA   | 49:u:414:VAL:HB   | 1.97                     | 0.46              |
| 49:u:685:GLN:O    | 49:u:689:LYS:N    | 2.49                     | 0.46              |
| 50:v:246:ILE:HD11 | 52:x:26:ARG:NH1   | 2.30                     | 0.46              |
| 52:x:447:LEU:HB2  | 52:x:473:PRO:HG3  | 1.96                     | 0.46              |
| 9:A:164:A:OP1     | 27:S:83:CYS:N     | 2.43                     | 0.46              |
| 9:A:1204:A:OP1    | 20:L:117:ARG:HB2  | 2.15                     | 0.46              |
| 24:P:78:ALA:HB1   | 24:P:119:LEU:HG   | 1.98                     | 0.46              |
| 34:c:217:MET:HG2  | 34:c:229:THR:HG23 | 1.98                     | 0.46              |
| 42:n:61:SER:OG    | 42:n:62:GLU:N     | 2.48                     | 0.46              |
| 44:p:56:LYS:HA    | 44:p:59:LEU:CD2   | 2.46                     | 0.46              |
| 48:t:441:ILE:O    | 48:t:457:GLY:N    | 2.49                     | 0.46              |
| 49:u:567:ARG:HB3  | 49:u:572:ARG:HA   | 1.96                     | 0.46              |
| 53:y:792:LEU:HD21 | 53:y:807:LEU:HD21 | 1.98                     | 0.46              |
| 3:4:341:ALA:CB    | 7:8:329:ASN:HA    | 2.45                     | 0.46              |
| 5:6:344:LYS:HA    | 5:6:347:TRP:HB2   | 1.97                     | 0.46              |
| 9:A:508:A:H3'     | 9:A:509:OMG:H8    | 1.80                     | 0.46              |
| 9:A:874:G:H2'     | 9:A:875:A:C8      | 2.50                     | 0.46              |
| 9:A:1016:U:H4'    | 17:I:16:LEU:HD23  | 1.96                     | 0.46              |
| 11:C:11:ARG:HA    | 11:C:28:ALA:HB2   | 1.98                     | 0.46              |
| 11:C:181:CYS:SG   | 11:C:182:MET:N    | 2.87                     | 0.46              |
| 11:C:185:GLY:HA2  | 11:C:189:LEU:HD12 | 1.98                     | 0.46              |
| 26:R:120:PRO:HD3  | 26:R:137:LEU:HD11 | 1.97                     | 0.46              |
| 27:S:63:MET:HE2   | 27:S:100:CYS:HA   | 1.98                     | 0.46              |
| 30:Y:55:VAL:HA    | 30:Y:63:PHE:CE1   | 2.51                     | 0.46              |
| 37:f:82:TRP:CD1   | 37:f:82:TRP:H     | 2.31                     | 0.46              |
| 41:m:75:ASN:CG    | 41:m:127:TYR:HA   | 2.41                     | 0.46              |
| 49:u:567:ARG:HA   | 49:u:573:GLN:HG3  | 1.97                     | 0.46              |
| 5:6:43:ALA:HB1    | 5:6:47:GLU:H      | 1.81                     | 0.46              |
| 9:A:1283:C:H4'    | 9:A:1287:A:H5'    | 1.96                     | 0.46              |
| 9:A:1536:G:H2'    | 9:A:1537:A:C8     | 2.51                     | 0.46              |
| 9:A:1568:C:H5''   | 35:d:96:SER:HB2   | 1.98                     | 0.46              |
| 10:B:57:ASP:HB3   | 10:B:60:CYS:HB2   | 1.98                     | 0.46              |
| 11:C:166:THR:HB   | 11:C:168:LYS:HG2  | 1.98                     | 0.46              |
| 23:O:180:ASP:OD1  | 23:O:180:ASP:N    | 2.48                     | 0.46              |
| 34:c:109:LEU:H    | 34:c:124:SER:HA   | 1.81                     | 0.46              |
| 47:s:302:CYS:O    | 47:s:306:HIS:N    | 2.37                     | 0.46              |
| 50:v:347:ILE:HD13 | 53:y:823:SER:HB2  | 1.98                     | 0.46              |
| 3:4:301:ASP:O     | 3:4:305:GLY:N     | 2.41                     | 0.46              |
| 9:A:561:A:OP2     | 12:D:174:LYS:N    | 2.49                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:C:122:LYS:HB3  | 11:C:162:ILE:HB   | 1.98                     | 0.46              |
| 11:C:125:LYS:HB3  | 11:C:142:HIS:HB3  | 1.98                     | 0.46              |
| 16:H:79:PHE:CE1   | 52:x:79:SER:HB3   | 2.50                     | 0.46              |
| 27:S:85:ARG:NH1   | 28:T:118:ARG:HD2  | 2.31                     | 0.46              |
| 30:Y:32:ILE:HA    | 30:Y:68:ILE:O     | 2.16                     | 0.46              |
| 34:c:234:ASP:H    | 34:c:252:THR:HB   | 1.81                     | 0.46              |
| 37:f:28:PHE:HE2   | 37:f:38:ARG:HD3   | 1.80                     | 0.46              |
| 40:k:125:GLU:H    | 40:k:125:GLU:HG3  | 1.43                     | 0.46              |
| 45:q:79:VAL:HG12  | 45:q:91:VAL:HG13  | 1.99                     | 0.46              |
| 46:r:200:TYR:CE1  | 48:t:343:ILE:CA   | 2.99                     | 0.46              |
| 47:s:195:VAL:HG11 | 48:t:194:LEU:C    | 2.41                     | 0.46              |
| 49:u:171:GLU:HA   | 49:u:174:TYR:HB3  | 1.98                     | 0.46              |
| 2:3:154:ASP:O     | 2:3:158:LEU:N     | 2.43                     | 0.45              |
| 9:A:54:A:H5'      | 28:T:108:LYS:NZ   | 2.31                     | 0.45              |
| 9:A:441:C:O2'     | 27:S:92:ARG:NH2   | 2.47                     | 0.45              |
| 11:C:73:ASP:HB3   | 11:C:145:ARG:NH2  | 2.31                     | 0.45              |
| 11:C:179:ASN:O    | 11:C:195:ILE:HG13 | 2.15                     | 0.45              |
| 18:J:96:SER:OG    | 18:J:97:ARG:N     | 2.49                     | 0.45              |
| 31:Z:40:ARG:NH1   | 31:Z:47:GLU:OE1   | 2.46                     | 0.45              |
| 35:d:60:THR:HA    | 35:d:63:HIS:HB2   | 1.98                     | 0.45              |
| 41:m:12:MET:HG2   | 41:m:119:GLN:HG2  | 1.97                     | 0.45              |
| 43:o:300:VAL:HG13 | 43:o:312:VAL:HG11 | 1.98                     | 0.45              |
| 47:s:231:ARG:HH11 | 47:s:235:HIS:HB3  | 1.81                     | 0.45              |
| 2:3:9:ALA:O       | 2:3:13:LYS:N      | 2.43                     | 0.45              |
| 3:4:341:ALA:HB1   | 7:8:329:ASN:CB    | 2.46                     | 0.45              |
| 9:A:1134:G:H5'    | 9:A:1135:C:OP2    | 2.15                     | 0.45              |
| 9:A:1587:G:N7     | 35:d:67:ARG:HD3   | 2.30                     | 0.45              |
| 24:P:34:PHE:O     | 24:P:41:PHE:N     | 2.46                     | 0.45              |
| 25:Q:23:CYS:SG    | 25:Q:74:CYS:N     | 2.90                     | 0.45              |
| 27:S:46:LYS:HE3   | 27:S:46:LYS:HB3   | 1.78                     | 0.45              |
| 29:V:47:LYS:HD3   | 30:Y:115:TYR:CZ   | 2.51                     | 0.45              |
| 30:Y:123:ASP:OD1  | 30:Y:125:ARG:HG3  | 2.17                     | 0.45              |
| 41:m:51:VAL:HB    | 41:m:77:ILE:HB    | 1.97                     | 0.45              |
| 3:4:89:GLY:C      | 5:6:100:SER:CB    | 2.89                     | 0.45              |
| 9:A:11:A:O2'      | 9:A:12:U:H5'      | 2.16                     | 0.45              |
| 9:A:116:OMU:O5'   | 9:A:116:OMU:H6    | 2.16                     | 0.45              |
| 9:A:223:C:H2'     | 9:A:224:A:C8      | 2.51                     | 0.45              |
| 9:A:830:A:OP2     | 9:A:846:G:N2      | 2.49                     | 0.45              |
| 9:A:874:G:H2'     | 9:A:875:A:H8      | 1.80                     | 0.45              |
| 9:A:1329:U:O2'    | 9:A:1332:A:OP2    | 2.25                     | 0.45              |
| 9:A:1822:A:H5'    | 9:A:1823:A:P      | 2.56                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 21:M:61:ILE:HA    | 21:M:61:ILE:HD13  | 1.65                     | 0.45              |
| 23:O:72:ALA:HB3   | 24:P:128:ARG:NH1  | 2.31                     | 0.45              |
| 24:P:103:ASN:OD1  | 24:P:103:ASN:N    | 2.46                     | 0.45              |
| 33:b:17:TYR:HB3   | 33:b:25:LEU:HD11  | 1.98                     | 0.45              |
| 42:n:36:ASP:OD1   | 52:x:481:ASN:ND2  | 2.50                     | 0.45              |
| 47:s:214:THR:O    | 47:s:261:ARG:NH1  | 2.47                     | 0.45              |
| 1:1:288:LYS:HA    | 1:1:362:GLY:N     | 2.30                     | 0.45              |
| 9:A:957:A:OP1     | 24:P:57:THR:CG2   | 2.64                     | 0.45              |
| 9:A:1399:C:H5''   | 34:c:100:ARG:NH2  | 2.32                     | 0.45              |
| 9:A:1519:U:H1'    | 37:f:135:HIS:NE2  | 2.30                     | 0.45              |
| 11:C:100:ARG:HH22 | 11:C:122:LYS:HA   | 1.81                     | 0.45              |
| 15:G:52:GLU:HA    | 15:G:58:LYS:HG3   | 1.97                     | 0.45              |
| 16:H:21:LYS:HD3   | 17:I:15:ALA:HB2   | 1.97                     | 0.45              |
| 22:N:119:PRO:HG2  | 22:N:142:LEU:HD11 | 1.99                     | 0.45              |
| 24:P:66:ARG:HH22  | 46:r:53:ARG:HB3   | 1.81                     | 0.45              |
| 32:a:74:GLU:H     | 32:a:74:GLU:HG3   | 1.48                     | 0.45              |
| 49:u:399:ASN:HB3  | 49:u:402:LYS:HZ3  | 1.82                     | 0.45              |
| 49:u:483:ARG:NH1  | 53:y:800:ASP:OD1  | 2.49                     | 0.45              |
| 8:9:1:MET:HE2     | 8:9:6:ARG:HA      | 1.98                     | 0.45              |
| 9:A:3:C:O4'       | 20:L:206:SER:C    | 2.59                     | 0.45              |
| 9:A:522:A:H5''    | 12:D:145:PRO:HD2  | 1.97                     | 0.45              |
| 9:A:802:A:N6      | 15:G:106:ARG:NH1  | 2.57                     | 0.45              |
| 9:A:841:G:OP2     | 28:T:14:THR:CB    | 2.64                     | 0.45              |
| 11:C:192:ILE:HG23 | 11:C:228:ILE:HD11 | 1.98                     | 0.45              |
| 13:E:46:HIS:HB3   | 13:E:101:LEU:HD11 | 1.98                     | 0.45              |
| 32:a:53:LYS:HB3   | 32:a:53:LYS:HE3   | 1.60                     | 0.45              |
| 35:d:138:VAL:O    | 35:d:142:ASN:N    | 2.50                     | 0.45              |
| 39:i:23:VAL:HB    | 39:i:42:CYS:SG    | 2.57                     | 0.45              |
| 40:k:141:CYS:CB   | 40:k:147:THR:HA   | 2.40                     | 0.45              |
| 41:m:72:HIS:HB2   | 41:m:74:ILE:HG13  | 1.97                     | 0.45              |
| 3:4:356:ASN:HA    | 7:8:313:ARG:CB    | 2.46                     | 0.45              |
| 9:A:1096:G:C8     | 9:A:1148:A:C6     | 3.05                     | 0.45              |
| 9:A:1255:G:O4'    | 38:h:71:GLY:HA3   | 2.17                     | 0.45              |
| 9:A:1692:U:H2'    | 9:A:1693:G:C8     | 2.51                     | 0.45              |
| 10:B:115:PRO:O    | 10:B:118:ARG:HG3  | 2.17                     | 0.45              |
| 15:G:100:ILE:HG12 | 15:G:125:VAL:HG21 | 1.98                     | 0.45              |
| 21:M:20:TYR:CZ    | 21:M:38:ILE:HB    | 2.51                     | 0.45              |
| 49:u:280:SER:OG   | 49:u:321:ARG:NH1  | 2.50                     | 0.45              |
| 53:y:391:THR:O    | 53:y:457:LYS:NZ   | 2.46                     | 0.45              |
| 9:A:121:OMU:HM23  | 9:A:121:OMU:H1'   | 1.84                     | 0.45              |
| 9:A:575:A:P       | 28:T:93:ARG:HH21  | 2.39                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:A:999:G:OP2     | 25:Q:17:HIS:HB2   | 2.17                     | 0.45              |
| 9:A:1171:G:O2'    | 9:A:1187:G:O6     | 2.29                     | 0.45              |
| 9:A:1264:C:N4     | 9:A:1518:C:N3     | 2.56                     | 0.45              |
| 11:C:69:PHE:CD2   | 28:T:17:LEU:HD22  | 2.51                     | 0.45              |
| 20:L:94:ILE:HG21  | 20:L:162:ILE:HD12 | 1.99                     | 0.45              |
| 29:V:16:ASP:OD1   | 29:V:16:ASP:N     | 2.50                     | 0.45              |
| 44:p:112:GLY:HA3  | 47:s:273:ARG:NH2  | 2.32                     | 0.45              |
| 46:r:127:LEU:HA   | 46:r:130:LEU:HB2  | 1.98                     | 0.45              |
| 49:u:500:ALA:HB1  | 49:u:502:ARG:HB2  | 1.99                     | 0.45              |
| 50:v:367:ALA:O    | 50:v:371:ILE:HG12 | 2.16                     | 0.45              |
| 51:w:2:G:O5'      | 51:w:2:G:H8       | 2.00                     | 0.45              |
| 1:1:528:VAL:HB    | 1:1:545:GLU:HB2   | 1.98                     | 0.45              |
| 1:1:530:VAL:HB    | 1:1:543:ASN:HB2   | 1.98                     | 0.45              |
| 3:4:124:VAL:HA    | 3:4:129:VAL:HA    | 1.99                     | 0.45              |
| 8:9:21:ARG:HD2    | 9:A:1717:C:O3'    | 2.17                     | 0.45              |
| 9:A:746:C:N4      | 9:A:797:C:O2      | 2.49                     | 0.45              |
| 9:A:919:A:OP1     | 17:I:20:ARG:HD2   | 2.17                     | 0.45              |
| 9:A:1228:A:H2'    | 9:A:1229:G:C8     | 2.52                     | 0.45              |
| 9:A:1337:C:H2'    | 9:A:1338:G:C8     | 2.52                     | 0.45              |
| 9:A:1705:C:H2'    | 9:A:1706:G:C8     | 2.52                     | 0.45              |
| 12:D:93:LYS:HB2   | 12:D:96:TYR:HD2   | 1.81                     | 0.45              |
| 13:E:123:VAL:HG12 | 13:E:124:LYS:HG3  | 1.98                     | 0.45              |
| 16:H:51:GLN:CD    | 17:I:55:ARG:HH22  | 2.25                     | 0.45              |
| 22:N:89:LYS:HG3   | 22:N:201:LEU:O    | 2.16                     | 0.45              |
| 23:O:28:LYS:HD3   | 23:O:48:LEU:HD13  | 1.99                     | 0.45              |
| 33:b:25:LEU:HD22  | 33:b:87:PRO:HG3   | 1.99                     | 0.45              |
| 46:r:32:ALA:HB2   | 46:r:63:ILE:CD1   | 2.46                     | 0.45              |
| 46:r:230:ILE:HB   | 46:r:234:ARG:HG2  | 1.98                     | 0.45              |
| 47:s:183:VAL:HA   | 47:s:186:ILE:CG1  | 2.47                     | 0.45              |
| 51:w:13:C:H2'     | 51:w:14:A:H4'     | 1.98                     | 0.45              |
| 53:y:386:ASN:OD1  | 53:y:386:ASN:N    | 2.50                     | 0.45              |
| 5:6:324:LYS:H     | 49:u:448:GLN:H    | 1.65                     | 0.45              |
| 9:A:998:A:OP2     | 25:Q:16:GLY:HA3   | 2.16                     | 0.45              |
| 10:B:35:ARG:NH2   | 10:B:51:ILE:CB    | 2.79                     | 0.45              |
| 32:a:92:ALA:O     | 32:a:96:ARG:HB2   | 2.16                     | 0.45              |
| 42:n:32:VAL:HG11  | 42:n:56:LEU:HD12  | 1.99                     | 0.45              |
| 45:q:57:ARG:NH1   | 45:q:81:LEU:HD13  | 2.32                     | 0.45              |
| 49:u:233:ARG:HA   | 49:u:236:GLN:HB3  | 1.99                     | 0.45              |
| 49:u:329:ILE:O    | 49:u:434:ASN:ND2  | 2.42                     | 0.45              |
| 49:u:411:LEU:HD23 | 49:u:432:GLN:HG2  | 1.97                     | 0.45              |
| 1:1:566:ILE:HD11  | 1:1:582:GLY:O     | 2.16                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:A:944:A:H5''    | 24:P:134:PRO:CB   | 2.47                     | 0.45              |
| 12:D:64:ASP:OD1   | 12:D:64:ASP:N     | 2.48                     | 0.45              |
| 21:M:20:TYR:CE2   | 21:M:38:ILE:HB    | 2.52                     | 0.45              |
| 49:u:446:ILE:HG23 | 49:u:447:TYR:HD1  | 1.81                     | 0.45              |
| 50:v:339:PHE:HA   | 50:v:342:GLU:HB3  | 1.98                     | 0.45              |
| 7:8:49:ILE:O      | 7:8:53:TYR:N      | 2.50                     | 0.44              |
| 9:A:346:C:H5''    | 11:C:38:LEU:HB2   | 1.99                     | 0.44              |
| 9:A:984:C:H1'     | 24:P:138:ASP:CG   | 2.42                     | 0.44              |
| 9:A:1106:C:H5''   | 16:H:70:LYS:HG3   | 1.99                     | 0.44              |
| 9:A:1142:G:N2     | 9:A:1145:A:OP2    | 2.43                     | 0.44              |
| 9:A:1668:U:OP2    | 30:Y:141:TYR:OH   | 2.31                     | 0.44              |
| 11:C:19:MET:SD    | 11:C:108:ARG:HD2  | 2.58                     | 0.44              |
| 29:V:103:LEU:HD11 | 36:e:67:LEU:HD22  | 1.99                     | 0.44              |
| 30:Y:132:PHE:CG   | 38:h:77:TRP:HB2   | 2.52                     | 0.44              |
| 34:c:230:LEU:HD13 | 34:c:259:TRP:CG   | 2.52                     | 0.44              |
| 40:k:138:ARG:HB2  | 40:k:150:PHE:N    | 2.29                     | 0.44              |
| 46:r:193:ALA:HB2  | 46:r:275:PRO:HA   | 1.98                     | 0.44              |
| 47:s:246:THR:HB   | 47:s:247:SER:H    | 1.62                     | 0.44              |
| 8:9:3:ALA:HB3     | 9:A:1842:C:OP1    | 2.17                     | 0.44              |
| 9:A:547:G:H8      | 9:A:547:G:H2'     | 1.64                     | 0.44              |
| 9:A:580:U:H2'     | 9:A:581:U:C6      | 2.52                     | 0.44              |
| 9:A:1452:A:O2'    | 9:A:1475:G:N2     | 2.50                     | 0.44              |
| 9:A:1598:G:OP1    | 36:e:80:ARG:NH2   | 2.47                     | 0.44              |
| 9:A:1824:A:H1'    | 45:q:45:GLY:CA    | 2.45                     | 0.44              |
| 23:O:101:HIS:ND1  | 23:O:101:HIS:O    | 2.50                     | 0.44              |
| 23:O:128:LYS:HE3  | 53:y:307:GLY:O    | 2.18                     | 0.44              |
| 26:R:61:ASP:OD1   | 26:R:61:ASP:N     | 2.49                     | 0.44              |
| 34:c:154:VAL:HG23 | 34:c:167:SER:HB3  | 1.99                     | 0.44              |
| 49:u:320:THR:HG21 | 49:u:384:VAL:HG23 | 1.99                     | 0.44              |
| 50:v:265:LYS:NZ   | 50:v:335:ASN:OD1  | 2.39                     | 0.44              |
| 9:A:54:A:OP1      | 28:T:111:LYS:NZ   | 2.44                     | 0.44              |
| 9:A:352:U:C5'     | 10:B:139:ARG:HG2  | 2.42                     | 0.44              |
| 9:A:562:U:H2'     | 9:A:563:G:C8      | 2.52                     | 0.44              |
| 9:A:688:U:C6      | 15:G:122:LEU:CD1  | 3.00                     | 0.44              |
| 9:A:1101:U:H2'    | 9:A:1102:G:C8     | 2.52                     | 0.44              |
| 9:A:1405:A:H2'    | 9:A:1406:G:O4'    | 2.17                     | 0.44              |
| 9:A:1406:G:H2'    | 9:A:1407:U:C6     | 2.53                     | 0.44              |
| 9:A:1544:C:O2     | 30:Y:76:GLY:HA2   | 2.18                     | 0.44              |
| 22:N:127:PRO:HG2  | 22:N:152:SER:HB3  | 1.99                     | 0.44              |
| 23:O:57:ILE:HG23  | 23:O:59:SER:H     | 1.82                     | 0.44              |
| 26:R:199:LEU:HD23 | 26:R:199:LEU:HA   | 1.80                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 31:Z:82:GLY:C     | 31:Z:84:VAL:H     | 2.25                     | 0.44              |
| 49:u:205:LEU:HD11 | 49:u:259:LEU:HD21 | 1.98                     | 0.44              |
| 50:v:128:LEU:O    | 50:v:132:TYR:N    | 2.49                     | 0.44              |
| 5:6:224:LEU:O     | 5:6:342:PHE:CZ    | 2.71                     | 0.44              |
| 9:A:145:G:H2'     | 9:A:146:G:C8      | 2.53                     | 0.44              |
| 9:A:185:G:H1      | 9:A:214:U:H3      | 1.66                     | 0.44              |
| 9:A:197:U:O2'     | 9:A:198:U:H5'     | 2.17                     | 0.44              |
| 9:A:581:U:OP1     | 28:T:65:GLY:N     | 2.41                     | 0.44              |
| 9:A:1277:C:H2'    | 9:A:1278:A:H8     | 1.81                     | 0.44              |
| 9:A:1675:A:O3'    | 29:V:74:ASN:HB3   | 2.17                     | 0.44              |
| 11:C:160:ILE:HB   | 11:C:169:ILE:HG23 | 1.99                     | 0.44              |
| 37:f:26:ILE:HG12  | 37:f:59:LEU:HD11  | 2.00                     | 0.44              |
| 40:k:119:ARG:H    | 40:k:119:ARG:HG3  | 1.51                     | 0.44              |
| 49:u:341:LEU:HD11 | 49:u:347:ILE:HG13 | 2.00                     | 0.44              |
| 49:u:552:LEU:HA   | 49:u:555:THR:HB   | 2.00                     | 0.44              |
| 50:v:349:GLN:HE21 | 53:y:833:ALA:CB   | 2.31                     | 0.44              |
| 9:A:4:C:C1'       | 12:D:18:ARG:HH12  | 2.25                     | 0.44              |
| 15:G:81:ARG:HE    | 15:G:81:ARG:HB2   | 1.53                     | 0.44              |
| 18:J:30:CYS:HB2   | 18:J:61:ILE:HG13  | 1.98                     | 0.44              |
| 20:L:107:LEU:HD11 | 20:L:129:ALA:HB2  | 2.00                     | 0.44              |
| 27:S:22:ARG:HG2   | 27:S:25:ARG:HH21  | 1.81                     | 0.44              |
| 28:T:41:ARG:NH1   | 28:T:52:PRO:O     | 2.44                     | 0.44              |
| 44:p:54:TYR:HE1   | 44:p:102:LEU:HD11 | 1.82                     | 0.44              |
| 46:r:155:HIS:O    | 46:r:159:ASP:N    | 2.47                     | 0.44              |
| 49:u:342:LEU:HA   | 49:u:346:GLY:HA2  | 1.99                     | 0.44              |
| 52:x:394:LYS:HD2  | 52:x:447:LEU:HD11 | 1.99                     | 0.44              |
| 9:A:583:A:H2'     | 9:A:584:A:H8      | 1.81                     | 0.44              |
| 9:A:683:OMG:H1'   | 9:A:683:OMG:HM23  | 1.78                     | 0.44              |
| 9:A:860:G:N2      | 18:J:107:SER:OG   | 2.37                     | 0.44              |
| 11:C:118:GLU:HA   | 11:C:121:TYR:CE2  | 2.53                     | 0.44              |
| 20:L:180:VAL:HG22 | 20:L:219:ILE:HD13 | 1.99                     | 0.44              |
| 22:N:52:LYS:HB3   | 22:N:52:LYS:HE2   | 1.89                     | 0.44              |
| 50:v:233:ILE:HD11 | 50:v:273:VAL:HB   | 1.99                     | 0.44              |
| 51:w:28:G:C2      | 51:w:41:A:C2      | 3.06                     | 0.44              |
| 52:x:34:SER:OG    | 52:x:57:ASN:OD1   | 2.36                     | 0.44              |
| 52:x:305:SER:O    | 52:x:308:SER:OG   | 2.34                     | 0.44              |
| 53:y:439:ARG:HH22 | 53:y:441:ARG:HH21 | 1.65                     | 0.44              |
| 53:y:475:ASP:OD1  | 53:y:475:ASP:N    | 2.49                     | 0.44              |
| 1:1:525:TYR:OH    | 1:1:548:ARG:NH2   | 2.50                     | 0.44              |
| 4:5:227:VAL:O     | 4:5:231:LEU:N     | 2.44                     | 0.44              |
| 9:A:2:A:C8        | 20:L:223:TYR:CD2  | 3.06                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:A:563:G:O6      | 12:D:172:ARG:NH2  | 2.50                     | 0.44              |
| 9:A:1101:U:OP1    | 23:O:151:ARG:HG2  | 2.18                     | 0.44              |
| 10:B:5:GLN:HG2    | 10:B:10:TYR:HA    | 1.99                     | 0.44              |
| 11:C:44:LEU:HB3   | 11:C:80:ILE:O     | 2.18                     | 0.44              |
| 23:O:108:ASP:O    | 25:Q:68:TYR:HE2   | 2.01                     | 0.44              |
| 26:R:201:LYS:HA   | 26:R:201:LYS:HD2  | 1.77                     | 0.44              |
| 34:c:5:MET:SD     | 34:c:270:LEU:HD21 | 2.58                     | 0.44              |
| 34:c:57:ARG:HD3   | 34:c:95:GLY:HA3   | 2.00                     | 0.44              |
| 40:k:99:LYS:HD3   | 40:k:99:LYS:HA    | 1.80                     | 0.44              |
| 45:q:57:ARG:HH12  | 45:q:81:LEU:HD13  | 1.81                     | 0.44              |
| 49:u:87:GLU:HG2   | 49:u:170:VAL:HG23 | 1.99                     | 0.44              |
| 49:u:91:ARG:HE    | 49:u:91:ARG:HB2   | 1.56                     | 0.44              |
| 50:v:261:VAL:HG21 | 50:v:274:LEU:HG   | 1.99                     | 0.44              |
| 50:v:349:GLN:CB   | 53:y:833:ALA:HB1  | 2.47                     | 0.44              |
| 1:1:549:MET:HA    | 1:1:554:VAL:HG13  | 2.00                     | 0.44              |
| 5:6:186:VAL:O     | 5:6:190:GLY:N     | 2.50                     | 0.44              |
| 9:A:307:G:O6      | 26:R:44:HIS:CE1   | 2.70                     | 0.44              |
| 9:A:798:G:C4      | 15:G:107:LYS:C    | 2.96                     | 0.44              |
| 9:A:1016:U:O2     | 17:I:17:PRO:HD2   | 2.17                     | 0.44              |
| 9:A:1122:A:C5'    | 23:O:205:TYR:CD2  | 3.00                     | 0.44              |
| 9:A:1588:A:H2'    | 9:A:1589:A:C8     | 2.52                     | 0.44              |
| 21:M:20:TYR:CE1   | 21:M:23:ARG:NH2   | 2.84                     | 0.44              |
| 24:P:74:ALA:HB1   | 24:P:115:ALA:HB2  | 1.99                     | 0.44              |
| 27:S:44:GLU:H     | 27:S:44:GLU:HG2   | 1.52                     | 0.44              |
| 44:p:54:TYR:OH    | 44:p:59:LEU:HB3   | 2.18                     | 0.44              |
| 44:p:91:LYS:HA    | 44:p:91:LYS:HD3   | 1.75                     | 0.44              |
| 46:r:167:ASP:OD1  | 46:r:167:ASP:N    | 2.51                     | 0.44              |
| 53:y:806:THR:O    | 53:y:810:MET:N    | 2.43                     | 0.44              |
| 9:A:377:G:OP1     | 26:R:98:LYS:HE2   | 2.17                     | 0.44              |
| 9:A:582:U:O2'     | 9:A:583:A:H5'     | 2.18                     | 0.44              |
| 9:A:642:U:H5      | 14:F:108:ARG:NH2  | 2.16                     | 0.44              |
| 9:A:921:G:H5'     | 16:H:21:LYS:HZ1   | 1.81                     | 0.44              |
| 9:A:1495:G:C8     | 39:i:41:GLN:HG2   | 2.53                     | 0.44              |
| 9:A:1615:U:H3     | 33:b:40:ARG:NH2   | 2.14                     | 0.44              |
| 9:A:1839:U:C4     | 9:A:1862:G:N1     | 2.86                     | 0.44              |
| 20:L:267:GLN:HG3  | 22:N:120:ARG:HH22 | 1.83                     | 0.44              |
| 24:P:146:ARG:C    | 24:P:148:GLY:N    | 2.73                     | 0.44              |
| 26:R:110:ARG:HD3  | 26:R:123:ARG:HH21 | 1.82                     | 0.44              |
| 28:T:12:PHE:CZ    | 28:T:21:LYS:HB3   | 2.52                     | 0.44              |
| 47:s:243:GLU:O    | 47:s:244:LEU:HB2  | 2.17                     | 0.44              |
| 52:x:381:MET:HB2  | 52:x:391:ILE:HD13 | 1.99                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:4:304:VAL:O     | 49:u:538:LYS:HG2  | 2.18                     | 0.43              |
| 9:A:1351:G:H4'    | 22:N:109:THR:CB   | 2.48                     | 0.43              |
| 10:B:42:LEU:HD13  | 10:B:72:ILE:HD11  | 2.00                     | 0.43              |
| 11:C:14:ALA:HB1   | 11:C:18:TRP:CE3   | 2.53                     | 0.43              |
| 11:C:139:LEU:HB3  | 11:C:147:ILE:HB   | 2.00                     | 0.43              |
| 16:H:7:LEU:HD12   | 18:J:24:GLN:HB3   | 2.00                     | 0.43              |
| 23:O:82:ARG:HH11  | 23:O:191:ASP:HB3  | 1.83                     | 0.43              |
| 27:S:53:SER:O     | 27:S:53:SER:OG    | 2.35                     | 0.43              |
| 31:Z:26:THR:HA    | 31:Z:34:TYR:CD2   | 2.53                     | 0.43              |
| 35:d:116:ASP:OD1  | 35:d:117:GLN:N    | 2.46                     | 0.43              |
| 46:r:74:ILE:HG22  | 46:r:75:ARG:HG3   | 2.00                     | 0.43              |
| 53:y:750:LYS:HD2  | 53:y:750:LYS:HA   | 1.74                     | 0.43              |
| 9:A:322:C:N4      | 9:A:323:C:O2      | 2.51                     | 0.43              |
| 9:A:380:G:OP1     | 26:R:31:ARG:HD2   | 2.18                     | 0.43              |
| 9:A:897:U:N3      | 9:A:899:U:O4      | 2.51                     | 0.43              |
| 9:A:1030:A:H2'    | 9:A:1031:A2M:H8   | 2.00                     | 0.43              |
| 9:A:1648:G:H5''   | 30:Y:125:ARG:CG   | 2.47                     | 0.43              |
| 9:A:1661:A:H8     | 39:i:14:PHE:HB2   | 1.80                     | 0.43              |
| 11:C:181:CYS:N    | 11:C:193:GLY:O    | 2.50                     | 0.43              |
| 16:H:57:VAL:HG22  | 16:H:60:SER:HB3   | 2.01                     | 0.43              |
| 49:u:10:ASN:HA    | 49:u:13:LYS:HD2   | 2.00                     | 0.43              |
| 7:8:212:ASN:O     | 7:8:216:TRP:N     | 2.49                     | 0.43              |
| 9:A:116:OMU:HN3   | 9:A:347:G:H1      | 1.66                     | 0.43              |
| 9:A:129:C:H4'     | 9:A:130:G:H5'     | 2.00                     | 0.43              |
| 9:A:174:OMC:HM23  | 9:A:174:OMC:H1'   | 1.81                     | 0.43              |
| 9:A:920:A:O2'     | 9:A:922:A:OP1     | 2.32                     | 0.43              |
| 9:A:1047:C:H5'    | 24:P:143:LYS:CB   | 2.47                     | 0.43              |
| 9:A:1387:G:N2     | 21:M:8:THR:HG21   | 2.33                     | 0.43              |
| 16:H:20:LYS:HA    | 16:H:23:ARG:NH1   | 2.33                     | 0.43              |
| 21:M:86:PRO:HG2   | 22:N:200:ASP:HB3  | 2.00                     | 0.43              |
| 27:S:2:LYS:HB2    | 27:S:108:VAL:HG23 | 1.99                     | 0.43              |
| 29:V:139:VAL:HG11 | 42:n:47:LYS:HB2   | 2.01                     | 0.43              |
| 37:f:6:PRO:HG2    | 37:f:58:GLU:HG2   | 2.00                     | 0.43              |
| 45:q:100:ALA:O    | 45:q:104:LYS:N    | 2.50                     | 0.43              |
| 49:u:257:HIS:CD2  | 49:u:358:LEU:HA   | 2.53                     | 0.43              |
| 49:u:386:GLU:HG2  | 49:u:413:TRP:CG   | 2.52                     | 0.43              |
| 53:y:459:MET:HB3  | 53:y:672:PRO:HB3  | 2.00                     | 0.43              |
| 53:y:673:PHE:HA   | 53:y:676:HIS:ND1  | 2.33                     | 0.43              |
| 5:6:131:ALA:HB3   | 5:6:135:GLY:HA3   | 2.00                     | 0.43              |
| 9:A:65:C:O5'      | 27:S:174:PRO:HA   | 2.19                     | 0.43              |
| 9:A:113:G:H22     | 9:A:292:A:H2'     | 1.84                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:A:834:C:O2'     | 9:A:836:G:N1      | 2.51                     | 0.43              |
| 9:A:956:G:H4'     | 24:P:60:MET:HG2   | 2.00                     | 0.43              |
| 9:A:1292:C:H2'    | 9:A:1293:A:C8     | 2.54                     | 0.43              |
| 9:A:1377:U:C4     | 22:N:102:ARG:NH2  | 2.86                     | 0.43              |
| 9:A:1403:C:N4     | 9:A:1433:C:OP1    | 2.51                     | 0.43              |
| 11:C:93:ASP:C     | 11:C:96:GLY:H     | 2.26                     | 0.43              |
| 15:G:27:LEU:HD22  | 15:G:45:ILE:HD11  | 2.00                     | 0.43              |
| 15:G:90:LYS:HA    | 15:G:90:LYS:HD3   | 1.86                     | 0.43              |
| 31:Z:163:PRO:HA   | 31:Z:166:TYR:CZ   | 2.52                     | 0.43              |
| 34:c:153:CYS:HB3  | 34:c:198:VAL:HG12 | 1.99                     | 0.43              |
| 50:v:353:ILE:HG12 | 50:v:371:ILE:HG13 | 2.01                     | 0.43              |
| 53:y:499:VAL:HA   | 53:y:502:ILE:HG22 | 2.01                     | 0.43              |
| 53:y:726:LEU:HD12 | 53:y:726:LEU:HA   | 1.91                     | 0.43              |
| 5:6:154:TRP:O     | 5:6:158:THR:N     | 2.43                     | 0.43              |
| 5:6:317:ARG:HG2   | 49:u:398:PHE:HE1  | 1.83                     | 0.43              |
| 9:A:43:U:OP2      | 9:A:485:A:N6      | 2.51                     | 0.43              |
| 9:A:295:C:H2'     | 9:A:296:U:C6      | 2.53                     | 0.43              |
| 23:O:28:LYS:HA    | 23:O:50:THR:HA    | 2.00                     | 0.43              |
| 29:V:103:LEU:HG   | 36:e:67:LEU:HB2   | 2.00                     | 0.43              |
| 34:c:8:ARG:HD3    | 34:c:8:ARG:HA     | 1.80                     | 0.43              |
| 44:p:57:LYS:O     | 44:p:60:VAL:HG12  | 2.18                     | 0.43              |
| 50:v:322:ASP:HB3  | 50:v:325:LEU:HD12 | 1.99                     | 0.43              |
| 50:v:393:MET:N    | 50:v:393:MET:SD   | 2.92                     | 0.43              |
| 52:x:71:TYR:CZ    | 53:y:563:ARG:HD2  | 2.54                     | 0.43              |
| 5:6:260:LYS:O     | 5:6:262:PHE:N     | 2.50                     | 0.43              |
| 9:A:868:G:C5      | 15:G:115:LYS:HG2  | 2.53                     | 0.43              |
| 9:A:1031:A2M:HM'1 | 17:I:113:PHE:HA   | 2.00                     | 0.43              |
| 9:A:1630:A:O2'    | 37:f:103:LEU:HD22 | 2.17                     | 0.43              |
| 9:A:1707:U:H2'    | 9:A:1708:C:C6     | 2.53                     | 0.43              |
| 9:A:1857:G:N7     | 24:P:146:ARG:CD   | 2.81                     | 0.43              |
| 11:C:11:ARG:HD2   | 11:C:20:LEU:HD13  | 2.00                     | 0.43              |
| 12:D:122:SER:OG   | 12:D:123:ILE:N    | 2.52                     | 0.43              |
| 23:O:166:LYS:HE3  | 23:O:166:LYS:HB3  | 1.74                     | 0.43              |
| 24:P:43:HIS:CD2   | 24:P:55:ARG:HB3   | 2.53                     | 0.43              |
| 27:S:132:ARG:H    | 27:S:132:ARG:HG2  | 1.63                     | 0.43              |
| 34:c:254:PRO:HA   | 34:c:285:GLN:HA   | 2.00                     | 0.43              |
| 41:m:37:GLU:C     | 41:m:39:ALA:N     | 2.76                     | 0.43              |
| 46:r:9:TYR:OH     | 46:r:101:LYS:NZ   | 2.49                     | 0.43              |
| 46:r:45:MET:HE2   | 46:r:47:LEU:HD12  | 1.99                     | 0.43              |
| 49:u:279:VAL:HA   | 49:u:282:VAL:HG12 | 2.01                     | 0.43              |
| 50:v:231:ASN:HA   | 50:v:235:LEU:HB2  | 2.01                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 53:y:421:GLY:N    | 53:y:440:VAL:HG13 | 2.34                     | 0.43              |
| 9:A:392:A:H3'     | 9:A:393:U:C6      | 2.54                     | 0.43              |
| 9:A:934:G:H22     | 9:A:1008:A:H2     | 1.66                     | 0.43              |
| 9:A:1015:U:P      | 16:H:20:LYS:NZ    | 2.92                     | 0.43              |
| 9:A:1226:G:H5'    | 9:A:1227:G:OP2    | 2.19                     | 0.43              |
| 9:A:1556:A:C6     | 39:i:13:LYS:HA    | 2.53                     | 0.43              |
| 10:B:116:CYS:SG   | 10:B:117:PHE:N    | 2.92                     | 0.43              |
| 29:V:31:ASN:HB2   | 29:V:117:ILE:HD13 | 2.01                     | 0.43              |
| 30:Y:17:LYS:HB3   | 30:Y:18:THR:H     | 1.74                     | 0.43              |
| 31:Z:192:TRP:NE1  | 31:Z:201:LYS:O    | 2.43                     | 0.43              |
| 45:q:40:LYS:HA    | 45:q:40:LYS:HD2   | 1.77                     | 0.43              |
| 45:q:84:TYR:O     | 45:q:85:GLN:C     | 2.61                     | 0.43              |
| 49:u:416:GLU:O    | 49:u:425:GLN:NE2  | 2.52                     | 0.43              |
| 50:v:267:VAL:HG13 | 50:v:270:ARG:HG3  | 1.99                     | 0.43              |
| 53:y:580:SER:OG   | 53:y:623:GLN:OE1  | 2.37                     | 0.43              |
| 9:A:29:G:H4'      | 13:E:129:SER:OG   | 2.18                     | 0.43              |
| 9:A:167:G:O2'     | 27:S:131:ARG:NE   | 2.51                     | 0.43              |
| 9:A:307:G:O6      | 26:R:44:HIS:CD2   | 2.68                     | 0.43              |
| 9:A:1358:U:H2'    | 9:A:1359:U:C6     | 2.54                     | 0.43              |
| 9:A:1532:C:OP1    | 9:A:1604:G:O2'    | 2.30                     | 0.43              |
| 9:A:1678:A2M:HM'3 | 9:A:1678:A2M:H1'  | 1.83                     | 0.43              |
| 11:C:211:LYS:HG3  | 11:C:215:GLY:HA2  | 2.01                     | 0.43              |
| 20:L:178:HIS:ND1  | 20:L:221:ASP:OD2  | 2.52                     | 0.43              |
| 21:M:41:ILE:HG21  | 21:M:47:ARG:HA    | 1.99                     | 0.43              |
| 31:Z:45:ARG:HD2   | 31:Z:85:GLU:CG    | 2.49                     | 0.43              |
| 37:f:85:ASN:HD22  | 37:f:98:VAL:CG2   | 2.32                     | 0.43              |
| 46:r:210:GLU:HA   | 46:r:213:ARG:HB2  | 2.01                     | 0.43              |
| 47:s:296:ARG:HA   | 47:s:296:ARG:HD2  | 1.78                     | 0.43              |
| 49:u:228:MET:HE3  | 49:u:228:MET:HB2  | 1.88                     | 0.43              |
| 49:u:448:GLN:O    | 49:u:493:PHE:N    | 2.49                     | 0.43              |
| 49:u:515:PRO:O    | 49:u:520:ARG:NH2  | 2.52                     | 0.43              |
| 49:u:567:ARG:O    | 49:u:572:ARG:N    | 2.51                     | 0.43              |
| 53:y:815:LEU:HA   | 53:y:818:VAL:HG12 | 2.01                     | 0.43              |
| 9:A:522:A:H4'     | 12:D:131:ARG:NH1  | 2.33                     | 0.43              |
| 9:A:550:C:O2'     | 9:A:551:U:O4'     | 2.32                     | 0.43              |
| 9:A:572:U:H5'     | 28:T:60:PHE:O     | 2.18                     | 0.43              |
| 9:A:579:C:H2'     | 9:A:580:U:C6      | 2.54                     | 0.43              |
| 9:A:953:C:O4'     | 24:P:52:THR:HG23  | 2.19                     | 0.43              |
| 9:A:1031:A2M:HM'1 | 17:I:113:PHE:HB2  | 2.00                     | 0.43              |
| 9:A:1491:G:H2'    | 9:A:1492:U:C6     | 2.53                     | 0.43              |
| 9:A:1868:U:O2'    | 9:A:1869:A:H5'    | 2.19                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 15:G:44:ASN:OD1   | 15:G:44:ASN:N     | 2.51                     | 0.43              |
| 24:P:119:LEU:HD23 | 24:P:119:LEU:HA   | 1.83                     | 0.43              |
| 27:S:31:ARG:HB2   | 27:S:31:ARG:CZ    | 2.49                     | 0.43              |
| 33:b:111:MET:CB   | 37:f:117:ILE:HD11 | 2.49                     | 0.43              |
| 42:n:17:VAL:HA    | 42:n:30:VAL:HG12  | 1.99                     | 0.43              |
| 49:u:343:ASP:OD2  | 53:y:698:MET:HG2  | 2.19                     | 0.43              |
| 49:u:555:THR:HA   | 49:u:558:LEU:HB2  | 2.00                     | 0.43              |
| 50:v:246:ILE:HD11 | 52:x:26:ARG:NH2   | 2.34                     | 0.43              |
| 50:v:307:GLY:HA2  | 50:v:311:LYS:HB2  | 2.01                     | 0.43              |
| 52:x:315:GLU:O    | 52:x:319:ILE:HG12 | 2.18                     | 0.43              |
| 2:3:210:VAL:O     | 2:3:214:MET:N     | 2.49                     | 0.43              |
| 9:A:557:U:H2'     | 9:A:558:G:C8      | 2.53                     | 0.43              |
| 9:A:581:U:O2'     | 28:T:33:ALA:HA    | 2.19                     | 0.43              |
| 9:A:678:U:OP2     | 9:A:1026:C:N4     | 2.42                     | 0.43              |
| 9:A:1122:A:H5''   | 23:O:205:TYR:CD2  | 2.54                     | 0.43              |
| 29:V:50:PRO:HG2   | 29:V:90:VAL:HG13  | 2.01                     | 0.43              |
| 46:r:195:ILE:HD11 | 46:r:271:VAL:HA   | 2.01                     | 0.43              |
| 50:v:331:ASP:OD1  | 50:v:331:ASP:N    | 2.49                     | 0.43              |
| 4:5:387:HIS:O     | 4:5:391:ARG:N     | 2.39                     | 0.42              |
| 5:6:325:ILE:HA    | 49:u:449:SER:OG   | 2.18                     | 0.42              |
| 9:A:1808:U:H2'    | 9:A:1809:A:C8     | 2.54                     | 0.42              |
| 10:B:35:ARG:H     | 10:B:35:ARG:HG3   | 1.57                     | 0.42              |
| 16:H:34:ASP:OD2   | 16:H:82:LYS:NZ    | 2.38                     | 0.42              |
| 17:I:69:ASN:HB3   | 17:I:73:ARG:NH2   | 2.34                     | 0.42              |
| 41:m:42:LEU:HD12  | 41:m:42:LEU:HA    | 1.92                     | 0.42              |
| 45:q:80:GLY:O     | 45:q:90:ASP:N     | 2.52                     | 0.42              |
| 9:A:932:G:OP1     | 23:O:157:GLN:HB3  | 2.18                     | 0.42              |
| 11:C:154:ILE:HG21 | 11:C:160:ILE:HG22 | 2.01                     | 0.42              |
| 11:C:192:ILE:H    | 11:C:243:GLY:HA3  | 1.84                     | 0.42              |
| 21:M:41:ILE:HG21  | 21:M:47:ARG:CA    | 2.48                     | 0.42              |
| 22:N:33:GLN:HE21  | 22:N:33:GLN:HB2   | 1.52                     | 0.42              |
| 41:m:38:ALA:HA    | 41:m:110:VAL:HG23 | 2.01                     | 0.42              |
| 41:m:72:HIS:HB2   | 41:m:74:ILE:HD11  | 2.01                     | 0.42              |
| 44:p:48:GLN:HG3   | 44:p:79:TYR:HB3   | 2.01                     | 0.42              |
| 44:p:110:VAL:C    | 44:p:112:GLY:N    | 2.75                     | 0.42              |
| 49:u:352:GLN:HG2  | 49:u:364:PRO:HB3  | 2.00                     | 0.42              |
| 53:y:439:ARG:HH12 | 53:y:441:ARG:HH21 | 1.68                     | 0.42              |
| 53:y:439:ARG:HH12 | 53:y:441:ARG:HE   | 1.67                     | 0.42              |
| 5:6:184:VAL:O     | 5:6:188:LEU:N     | 2.45                     | 0.42              |
| 5:6:324:LYS:HZ1   | 5:6:328:THR:HA    | 1.84                     | 0.42              |
| 9:A:750:C:N4      | 9:A:793:G:O2'     | 2.53                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:C:101:LEU:HD23 | 11:C:101:LEU:HA   | 1.76                     | 0.42              |
| 30:Y:134:GLY:HA3  | 30:Y:140:ARG:HA   | 2.00                     | 0.42              |
| 32:a:16:PHE:HB2   | 32:a:79:LEU:HD13  | 2.01                     | 0.42              |
| 34:c:275:ILE:HD12 | 34:c:275:ILE:HA   | 1.83                     | 0.42              |
| 45:q:78:LEU:HB3   | 45:q:93:LEU:HG    | 2.01                     | 0.42              |
| 47:s:243:GLU:HG2  | 47:s:270:VAL:HG13 | 2.01                     | 0.42              |
| 50:v:249:MET:HB2  | 50:v:281:ILE:HG12 | 2.00                     | 0.42              |
| 52:x:42:VAL:HG12  | 53:y:636:ILE:HG12 | 2.00                     | 0.42              |
| 1:1:586:ARG:HA    | 1:1:608:LYS:HA    | 2.01                     | 0.42              |
| 9:A:67:C:OP1      | 27:S:162:LEU:HD21 | 2.19                     | 0.42              |
| 9:A:384:U:O4      | 26:R:5:ARG:NH2    | 2.48                     | 0.42              |
| 9:A:614:C:H2'     | 9:A:626:G:C8      | 2.55                     | 0.42              |
| 9:A:851:C:H5''    | 9:A:852:G:H5'     | 2.00                     | 0.42              |
| 9:A:1262:C:H4'    | 39:i:10:HIS:CE1   | 2.55                     | 0.42              |
| 9:A:1680:G:H4'    | 42:n:20:ARG:CD    | 2.50                     | 0.42              |
| 11:C:149:TYR:HB3  | 27:S:209:TYR:HB2  | 2.01                     | 0.42              |
| 11:C:163:ASP:HB3  | 11:C:168:LYS:H    | 1.85                     | 0.42              |
| 15:G:144:ILE:HG23 | 15:G:154:ILE:HG12 | 2.02                     | 0.42              |
| 33:b:37:TYR:HE1   | 33:b:112:ILE:HG22 | 1.85                     | 0.42              |
| 41:m:52:LEU:HB2   | 41:m:76:LEU:HD21  | 2.00                     | 0.42              |
| 49:u:254:GLU:HG3  | 49:u:358:LEU:HD21 | 2.01                     | 0.42              |
| 52:x:448:LYS:HE3  | 52:x:448:LYS:HB3  | 1.73                     | 0.42              |
| 53:y:521:ARG:HD3  | 53:y:521:ARG:HA   | 1.86                     | 0.42              |
| 1:1:489:ILE:HA    | 1:1:490:PRO:HD2   | 1.83                     | 0.42              |
| 3:4:265:LEU:O     | 3:4:269:LEU:N     | 2.50                     | 0.42              |
| 9:A:67:C:H5       | 27:S:162:LEU:HB3  | 1.81                     | 0.42              |
| 9:A:1058:A:H1'    | 44:p:38:ARG:HD2   | 2.00                     | 0.42              |
| 9:A:1114:U:O2'    | 9:A:1119:A:N6     | 2.53                     | 0.42              |
| 9:A:1709:G:H2'    | 9:A:1710:C:C6     | 2.53                     | 0.42              |
| 16:H:36:LYS:N     | 16:H:78:SER:O     | 2.44                     | 0.42              |
| 21:M:109:LEU:HD12 | 21:M:109:LEU:HA   | 1.80                     | 0.42              |
| 22:N:184:ARG:NH1  | 22:N:191:ARG:O    | 2.52                     | 0.42              |
| 24:P:117:ARG:HA   | 25:Q:53:ILE:HD11  | 2.02                     | 0.42              |
| 30:Y:51:LEU:HD21  | 30:Y:81:ILE:HB    | 2.01                     | 0.42              |
| 31:Z:134:CYS:SG   | 31:Z:135:GLU:N    | 2.92                     | 0.42              |
| 37:f:45:LEU:HD23  | 37:f:45:LEU:HA    | 1.92                     | 0.42              |
| 40:k:138:ARG:CG   | 40:k:149:CYS:HA   | 2.48                     | 0.42              |
| 42:n:43:ILE:N     | 42:n:64:GLU:OE2   | 2.53                     | 0.42              |
| 45:q:42:LEU:HD12  | 45:q:42:LEU:HA    | 1.84                     | 0.42              |
| 45:q:86:ASP:HB3   | 45:q:87:ASN:H     | 1.67                     | 0.42              |
| 5:6:207:CYS:O     | 5:6:211:ALA:N     | 2.50                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:A:525:A:H5''    | 14:F:106:ALA:HB2  | 1.99                     | 0.42              |
| 9:A:692:G:H2'     | 9:A:693:A:C8      | 2.54                     | 0.42              |
| 9:A:1256:G:O6     | 38:h:65:THR:HG22  | 2.19                     | 0.42              |
| 15:G:132:ASP:OD1  | 15:G:132:ASP:N    | 2.53                     | 0.42              |
| 18:J:102:ILE:HB   | 18:J:113:HIS:HB3  | 2.02                     | 0.42              |
| 20:L:210:PRO:HB3  | 20:L:240:THR:HG21 | 2.02                     | 0.42              |
| 21:M:78:ARG:HH21  | 22:N:89:LYS:HZ2   | 1.67                     | 0.42              |
| 21:M:81:ARG:HA    | 21:M:81:ARG:NH2   | 2.34                     | 0.42              |
| 24:P:120:ALA:C    | 24:P:122:SER:N    | 2.76                     | 0.42              |
| 31:Z:99:ILE:HG23  | 31:Z:173:ARG:HH21 | 1.84                     | 0.42              |
| 41:m:61:TYR:CE1   | 41:m:107:SER:HB2  | 2.55                     | 0.42              |
| 47:s:195:VAL:HG21 | 48:t:195:VAL:O    | 2.19                     | 0.42              |
| 50:v:205:LEU:H    | 50:v:205:LEU:HG   | 1.35                     | 0.42              |
| 9:A:517:OMC:HM23  | 9:A:517:OMC:H1'   | 1.79                     | 0.42              |
| 9:A:642:U:OP2     | 12:D:39:ASN:HB2   | 2.20                     | 0.42              |
| 9:A:1016:U:H4'    | 17:I:16:LEU:CD2   | 2.50                     | 0.42              |
| 9:A:1406:G:N2     | 9:A:1443:C:H42    | 2.18                     | 0.42              |
| 12:D:137:VAL:HG22 | 12:D:157:ILE:HG12 | 2.01                     | 0.42              |
| 33:b:21:ASP:OD1   | 33:b:21:ASP:N     | 2.46                     | 0.42              |
| 37:f:35:GLY:HA3   | 37:f:99:LEU:HA    | 2.00                     | 0.42              |
| 45:q:65:LEU:HD22  | 45:q:68:LYS:HD2   | 2.02                     | 0.42              |
| 1:l:698:ARG:C     | 1:l:700:CYS:N     | 2.73                     | 0.42              |
| 9:A:60:G:H22      | 9:A:316:G:H21     | 1.67                     | 0.42              |
| 9:A:1283:C:C4'    | 9:A:1287:A:H5'    | 2.49                     | 0.42              |
| 9:A:1399:C:H5''   | 34:c:100:ARG:NH1  | 2.33                     | 0.42              |
| 9:A:1852:C:H2'    | 9:A:1853:C:C6     | 2.54                     | 0.42              |
| 9:A:1865:C:H5''   | 25:Q:92:ARG:O     | 2.19                     | 0.42              |
| 11:C:86:PHE:CZ    | 11:C:182:MET:HG2  | 2.55                     | 0.42              |
| 11:C:161:GLN:HB3  | 11:C:170:THR:CB   | 2.39                     | 0.42              |
| 23:O:214:LYS:HB2  | 23:O:214:LYS:HE3  | 1.91                     | 0.42              |
| 26:R:88:ASN:OD1   | 26:R:205:ARG:NH1  | 2.53                     | 0.42              |
| 30:Y:100:VAL:HG23 | 30:Y:101:ASP:N    | 2.34                     | 0.42              |
| 32:a:4:PRO:HB2    | 32:a:7:ASN:HB2    | 2.02                     | 0.42              |
| 37:f:88:LYS:HG3   | 37:f:95:TYR:CE1   | 2.54                     | 0.42              |
| 40:k:135:HIS:HB2  | 40:k:140:TYR:HB2  | 2.01                     | 0.42              |
| 49:u:562:ARG:O    | 49:u:566:GLN:NE2  | 2.52                     | 0.42              |
| 53:y:703:SER:O    | 53:y:703:SER:OG   | 2.32                     | 0.42              |
| 4:5:201:ARG:O     | 4:5:205:ALA:N     | 2.49                     | 0.42              |
| 5:6:309:GLU:HB3   | 49:u:447:TYR:OH   | 2.20                     | 0.42              |
| 9:A:96:C:O2       | 9:A:473:A:O2'     | 2.32                     | 0.42              |
| 9:A:928:G:H2'     | 9:A:929:G:C8      | 2.54                     | 0.42              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 9:A:931:C:H5''    | 23:O:157:GLN:OE1 | 2.20                     | 0.42              |
| 9:A:1229:G:OP1    | 37:f:142:ARG:HD2 | 2.19                     | 0.42              |
| 9:A:1350:U:O2     | 22:N:110:ASN:CG  | 2.63                     | 0.42              |
| 9:A:1441:U:H1'    | 9:A:1443:C:H41   | 1.84                     | 0.42              |
| 11:C:153:LEU:HD23 | 11:C:153:LEU:HA  | 1.79                     | 0.42              |
| 15:G:27:LEU:O     | 15:G:31:GLU:N    | 2.53                     | 0.42              |
| 21:M:27:ASP:HB3   | 21:M:30:THR:HB   | 2.02                     | 0.42              |
| 34:c:118:ARG:O    | 34:c:134:THR:OG1 | 2.36                     | 0.42              |
| 41:m:83:LYS:HB2   | 41:m:83:LYS:HE2  | 1.73                     | 0.42              |
| 46:r:168:LEU:HD13 | 46:r:172:GLU:HB3 | 2.02                     | 0.42              |
| 53:y:95:SER:OG    | 53:y:96:ILE:N    | 2.52                     | 0.42              |
| 53:y:113:LEU:HD12 | 53:y:113:LEU:HA  | 1.87                     | 0.42              |
| 1:1:288:LYS:CB    | 1:1:361:GLY:HA3  | 2.50                     | 0.42              |
| 3:4:118:GLY:N     | 3:4:173:TYR:O    | 2.53                     | 0.42              |
| 3:4:156:MET:CB    | 7:8:106:SER:CB   | 2.98                     | 0.42              |
| 3:4:341:ALA:HB1   | 7:8:329:ASN:CA   | 2.48                     | 0.42              |
| 4:5:194:PHE:HA    | 4:5:232:HIS:HA   | 2.01                     | 0.42              |
| 5:6:313:ILE:HA    | 5:6:316:VAL:HG12 | 2.01                     | 0.42              |
| 9:A:1674:G:H5''   | 29:V:86:LYS:HD2  | 2.01                     | 0.42              |
| 11:C:9:LEU:HD12   | 11:C:9:LEU:HA    | 1.84                     | 0.42              |
| 12:D:101:LYS:HA   | 12:D:101:LYS:HD3 | 1.73                     | 0.42              |
| 20:L:213:LEU:HD12 | 20:L:213:LEU:HA  | 1.87                     | 0.42              |
| 21:M:33:ARG:HD3   | 21:M:33:ARG:HA   | 1.89                     | 0.42              |
| 27:S:149:LYS:HD2  | 27:S:149:LYS:HA  | 1.85                     | 0.42              |
| 34:c:201:SER:HB3  | 34:c:206:LEU:HB2 | 2.01                     | 0.42              |
| 40:k:141:CYS:C    | 40:k:144:CYS:HB2 | 2.45                     | 0.42              |
| 41:m:94:ILE:HG23  | 41:m:97:GLU:O    | 2.20                     | 0.42              |
| 49:u:558:LEU:HA   | 49:u:561:SER:HB2 | 2.01                     | 0.42              |
| 50:v:223:PHE:HB3  | 50:v:224:ASN:H   | 1.74                     | 0.42              |
| 50:v:325:LEU:HD23 | 50:v:325:LEU:HA  | 1.83                     | 0.42              |
| 52:x:304:ASN:OD1  | 52:x:311:ASN:ND2 | 2.53                     | 0.42              |
| 53:y:70:ALA:HA    | 53:y:73:ILE:HG22 | 2.02                     | 0.42              |
| 7:8:41:ILE:HA     | 7:8:78:ILE:H     | 1.84                     | 0.41              |
| 9:A:116:OMU:HM23  | 9:A:116:OMU:H1'  | 1.78                     | 0.41              |
| 9:A:581:U:H2'     | 9:A:582:U:C6     | 2.55                     | 0.41              |
| 9:A:1272:C:N4     | 9:A:1508:A:OP1   | 2.53                     | 0.41              |
| 9:A:1749:G:H2'    | 9:A:1750:C:C6    | 2.55                     | 0.41              |
| 10:B:57:ASP:HB2   | 10:B:115:PRO:HG2 | 2.01                     | 0.41              |
| 15:G:73:GLN:HA    | 15:G:76:GLN:HB2  | 2.02                     | 0.41              |
| 23:O:62:LEU:HD13  | 23:O:91:VAL:HG11 | 2.02                     | 0.41              |
| 29:V:75:SER:O     | 29:V:75:SER:OG   | 2.34                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 31:Z:52:ALA:HB3   | 31:Z:55:THR:HG22  | 2.01                     | 0.41              |
| 50:v:208:LEU:O    | 50:v:212:THR:N    | 2.48                     | 0.41              |
| 3:4:106:TYR:O     | 49:u:569:LEU:HA   | 2.20                     | 0.41              |
| 9:A:1644:C:H2'    | 9:A:1645:C:C6     | 2.55                     | 0.41              |
| 9:A:1826:G:O4'    | 45:q:43:GLY:HA2   | 2.20                     | 0.41              |
| 18:J:42:MET:HE2   | 18:J:42:MET:HB3   | 1.90                     | 0.41              |
| 24:P:101:GLY:HA3  | 24:P:134:PRO:HG2  | 2.02                     | 0.41              |
| 24:P:142:ARG:NH2  | 25:Q:27:ALA:HB2   | 2.34                     | 0.41              |
| 27:S:221:LYS:HE3  | 27:S:221:LYS:HB3  | 1.84                     | 0.41              |
| 29:V:49:LEU:HD12  | 30:Y:50:LYS:HG2   | 2.02                     | 0.41              |
| 33:b:18:ARG:HE    | 37:f:88:LYS:HB3   | 1.86                     | 0.41              |
| 35:d:29:LYS:H     | 35:d:106:ALA:HB1  | 1.84                     | 0.41              |
| 42:n:13:ARG:N     | 42:n:33:GLU:O     | 2.46                     | 0.41              |
| 44:p:39:ASN:O     | 44:p:41:ARG:N     | 2.53                     | 0.41              |
| 44:p:43:THR:HG21  | 44:p:88:ASP:HB2   | 2.02                     | 0.41              |
| 44:p:56:LYS:O     | 44:p:59:LEU:HG    | 2.20                     | 0.41              |
| 45:q:69:VAL:HG22  | 45:q:94:LYS:HE3   | 2.03                     | 0.41              |
| 46:r:50:GLU:OE1   | 46:r:88:ARG:NH2   | 2.53                     | 0.41              |
| 49:u:407:VAL:HG22 | 49:u:411:LEU:HD13 | 2.00                     | 0.41              |
| 49:u:481:GLN:HG2  | 49:u:499:TYR:CD1  | 2.56                     | 0.41              |
| 53:y:83:PHE:HA    | 53:y:86:LEU:HB2   | 2.02                     | 0.41              |
| 53:y:458:ILE:HG22 | 53:y:459:MET:HE2  | 2.02                     | 0.41              |
| 53:y:552:CYS:HB3  | 53:y:556:TYR:CZ   | 2.55                     | 0.41              |
| 53:y:616:LEU:HD23 | 53:y:616:LEU:HA   | 1.91                     | 0.41              |
| 9:A:158:A:H61     | 9:A:467:G:H1'     | 1.85                     | 0.41              |
| 9:A:835:C:C4      | 28:T:8:ARG:HD2    | 2.55                     | 0.41              |
| 9:A:921:G:H21     | 16:H:22:LYS:NZ    | 2.17                     | 0.41              |
| 9:A:1099:G:H22    | 9:A:1133:A:H2     | 1.69                     | 0.41              |
| 9:A:1303:C:C4     | 9:A:1304:U:C4     | 3.08                     | 0.41              |
| 9:A:1695:A:N7     | 9:A:1833:C:H4'    | 2.35                     | 0.41              |
| 9:A:1751:C:O2'    | 9:A:1753:C:OP2    | 2.35                     | 0.41              |
| 9:A:1844:U:H2'    | 9:A:1845:A:C8     | 2.55                     | 0.41              |
| 11:C:143:ASP:O    | 11:C:144:ALA:HB3  | 2.20                     | 0.41              |
| 13:E:24:ASP:HB3   | 13:E:27:TYR:HB3   | 2.03                     | 0.41              |
| 20:L:114:LYS:HD3  | 20:L:121:ARG:NH2  | 2.35                     | 0.41              |
| 30:Y:30:GLY:HA2   | 30:Y:66:VAL:O     | 2.21                     | 0.41              |
| 44:p:39:ASN:O     | 44:p:42:LYS:HG2   | 2.20                     | 0.41              |
| 49:u:290:LEU:HA   | 49:u:329:ILE:HD13 | 2.02                     | 0.41              |
| 49:u:330:PRO:O    | 49:u:333:PRO:HD3  | 2.20                     | 0.41              |
| 49:u:483:ARG:N    | 49:u:492:SER:O    | 2.43                     | 0.41              |
| 51:w:34:A:H2'     | 51:w:35:U:H5'     | 2.02                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:4:93:ARG:O      | 3:4:130:GLU:HA    | 2.20                     | 0.41              |
| 9:A:159:A2M:HM'3  | 9:A:159:A2M:H1'   | 1.94                     | 0.41              |
| 9:A:1058:A:C6     | 9:A:1059:G:C6     | 3.08                     | 0.41              |
| 9:A:1282:A:H3'    | 9:A:1283:C:C6     | 2.55                     | 0.41              |
| 9:A:1404:U:C5     | 38:h:88:LEU:HD21  | 2.55                     | 0.41              |
| 9:A:1677:U:O4     | 9:A:1678:A2M:N6   | 2.53                     | 0.41              |
| 9:A:1736:G:H2'    | 9:A:1737:G:C8     | 2.56                     | 0.41              |
| 14:F:98:LYS:H     | 14:F:98:LYS:HD3   | 1.85                     | 0.41              |
| 15:G:36:LEU:HD11  | 15:G:78:ARG:HD2   | 2.01                     | 0.41              |
| 19:K:45:ARG:HB2   | 22:N:185:MET:O    | 2.20                     | 0.41              |
| 45:q:100:ALA:HA   | 45:q:103:LEU:HB2  | 2.01                     | 0.41              |
| 49:u:531:ALA:HA   | 49:u:534:LEU:HB3  | 2.03                     | 0.41              |
| 53:y:55:LYS:HE3   | 53:y:55:LYS:HB2   | 1.86                     | 0.41              |
| 9:A:202:G:H5'     | 26:R:143:LYS:HG2  | 2.02                     | 0.41              |
| 9:A:496:C:O2'     | 11:C:27:PHE:HB3   | 2.20                     | 0.41              |
| 9:A:960:U:OP2     | 24:P:38:ASN:ND2   | 2.52                     | 0.41              |
| 9:A:1221:G:H2'    | 9:A:1222:G:C8     | 2.55                     | 0.41              |
| 9:A:1226:G:C2     | 9:A:1641:A:C6     | 3.08                     | 0.41              |
| 9:A:1709:G:C6     | 9:A:1826:G:C6     | 3.08                     | 0.41              |
| 16:H:79:PHE:O     | 52:x:78:SER:HA    | 2.19                     | 0.41              |
| 29:V:76:MET:HE2   | 29:V:76:MET:HB2   | 1.96                     | 0.41              |
| 29:V:97:PHE:HA    | 29:V:100:ILE:HD12 | 2.03                     | 0.41              |
| 29:V:102:LEU:CD1  | 36:e:100:VAL:HG21 | 2.36                     | 0.41              |
| 32:a:73:ASN:O     | 32:a:76:ILE:HB    | 2.20                     | 0.41              |
| 41:m:52:LEU:HG    | 41:m:107:SER:O    | 2.21                     | 0.41              |
| 44:p:64:LYS:O     | 44:p:65:LYS:C     | 2.63                     | 0.41              |
| 48:t:158:LEU:HA   | 48:t:188:LEU:O    | 2.20                     | 0.41              |
| 52:x:72:PHE:HA    | 53:y:600:HIS:O    | 2.21                     | 0.41              |
| 5:6:292:ILE:HA    | 5:6:297:MET:CB    | 2.51                     | 0.41              |
| 8:9:10:MET:HE2    | 8:9:10:MET:HB2    | 1.99                     | 0.41              |
| 9:A:1253:A:O2'    | 9:A:1666:C:O3'    | 2.39                     | 0.41              |
| 12:D:129:LEU:HD23 | 12:D:129:LEU:HA   | 1.83                     | 0.41              |
| 19:K:1:MET:HE3    | 20:L:166:ARG:HH11 | 1.85                     | 0.41              |
| 30:Y:105:LYS:O    | 30:Y:108:ILE:HG12 | 2.20                     | 0.41              |
| 52:x:43:ALA:HB2   | 53:y:609:TYR:CD2  | 2.56                     | 0.41              |
| 2:3:174:MET:O     | 2:3:178:GLY:N     | 2.54                     | 0.41              |
| 9:A:29:G:H2'      | 9:A:30:C:C6       | 2.56                     | 0.41              |
| 11:C:81:THR:O     | 11:C:82:TYR:C     | 2.62                     | 0.41              |
| 13:E:130:LEU:HA   | 13:E:130:LEU:HD12 | 1.83                     | 0.41              |
| 23:O:74:LEU:HD23  | 23:O:74:LEU:HA    | 1.90                     | 0.41              |
| 24:P:118:ALA:C    | 24:P:120:ALA:N    | 2.79                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:S:63:MET:HG2   | 27:S:98:ARG:HD2   | 2.03                     | 0.41              |
| 31:Z:11:PHE:CE2   | 38:h:27:ARG:HG3   | 2.55                     | 0.41              |
| 33:b:56:LEU:HD22  | 33:b:80:LEU:HD12  | 2.01                     | 0.41              |
| 35:d:64:LEU:HD23  | 35:d:64:LEU:HA    | 1.93                     | 0.41              |
| 49:u:304:ARG:NH1  | 49:u:315:MET:SD   | 2.94                     | 0.41              |
| 51:w:33:C:H2'     | 51:w:34:A:O4'     | 2.21                     | 0.41              |
| 3:4:288:GLN:CB    | 5:6:348:GLN:HE21  | 2.34                     | 0.41              |
| 9:A:65:C:C5       | 27:S:174:PRO:HB3  | 2.56                     | 0.41              |
| 9:A:580:U:H2'     | 9:A:581:U:H6      | 1.86                     | 0.41              |
| 9:A:640:A:H2'     | 9:A:641:A:C8      | 2.56                     | 0.41              |
| 9:A:1298:G:H1'    | 33:b:79:HIS:CD2   | 2.55                     | 0.41              |
| 9:A:1714:U:H2'    | 9:A:1715:A:C8     | 2.54                     | 0.41              |
| 20:L:213:LEU:HD23 | 20:L:240:THR:HG23 | 2.03                     | 0.41              |
| 20:L:230:THR:H    | 20:L:230:THR:HG22 | 1.63                     | 0.41              |
| 21:M:76:GLU:O     | 21:M:79:GLU:N     | 2.46                     | 0.41              |
| 26:R:203:LYS:HE3  | 26:R:203:LYS:HB2  | 1.80                     | 0.41              |
| 32:a:19:GLY:HA3   | 32:a:93:THR:OG1   | 2.20                     | 0.41              |
| 33:b:96:VAL:O     | 33:b:103:ASN:N    | 2.52                     | 0.41              |
| 47:s:214:THR:HA   | 47:s:261:ARG:HH11 | 1.86                     | 0.41              |
| 48:t:159:ILE:O    | 48:t:189:GLN:HA   | 2.21                     | 0.41              |
| 49:u:510:HIS:ND1  | 49:u:511:LEU:HG   | 2.36                     | 0.41              |
| 1:1:562:LYS:HA    | 1:1:562:LYS:HD2   | 1.90                     | 0.41              |
| 2:3:173:TRP:O     | 2:3:177:TYR:N     | 2.52                     | 0.41              |
| 9:A:399:C:O2      | 10:B:106:HIS:HB3  | 2.20                     | 0.41              |
| 9:A:556:U:H3'     | 9:A:557:U:H5''    | 2.01                     | 0.41              |
| 9:A:585:C:H2'     | 9:A:586:G:H8      | 1.84                     | 0.41              |
| 9:A:848:U:H2'     | 9:A:849:A:C8      | 2.56                     | 0.41              |
| 9:A:897:U:H5'     | 9:A:898:U:O4'     | 2.21                     | 0.41              |
| 9:A:1189:A:H2'    | 9:A:1190:A:C8     | 2.56                     | 0.41              |
| 9:A:1377:U:N3     | 22:N:102:ARG:CZ   | 2.83                     | 0.41              |
| 9:A:1543:U:P      | 35:d:62:ARG:HH22  | 2.43                     | 0.41              |
| 11:C:127:ARG:NE   | 11:C:142:HIS:HA   | 2.35                     | 0.41              |
| 11:C:192:ILE:N    | 11:C:243:GLY:HA3  | 2.36                     | 0.41              |
| 14:F:80:LEU:HA    | 14:F:80:LEU:HD13  | 1.81                     | 0.41              |
| 15:G:168:HIS:CE1  | 15:G:169:LYS:HE2  | 2.56                     | 0.41              |
| 19:K:69:ILE:HD13  | 19:K:69:ILE:HA    | 1.92                     | 0.41              |
| 20:L:82:TYR:CZ    | 20:L:164:PRO:HD3  | 2.56                     | 0.41              |
| 20:L:183:LYS:HG2  | 20:L:197:PRO:HD2  | 2.02                     | 0.41              |
| 21:M:34:VAL:HG22  | 34:c:150:TRP:HH2  | 1.83                     | 0.41              |
| 25:Q:79:ILE:HG21  | 25:Q:79:ILE:HD13  | 1.89                     | 0.41              |
| 26:R:158:ILE:HD12 | 26:R:158:ILE:HA   | 1.80                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 27:S:128:THR:OG1  | 27:S:129:VAL:N    | 2.53                     | 0.41              |
| 31:Z:161:GLY:C    | 31:Z:163:PRO:HD2  | 2.46                     | 0.41              |
| 33:b:44:ARG:NH2   | 33:b:82:ASP:O     | 2.54                     | 0.41              |
| 34:c:31:ILE:HG23  | 34:c:45:LEU:HD11  | 2.02                     | 0.41              |
| 37:f:79:ILE:HA    | 37:f:80:PRO:HD3   | 1.96                     | 0.41              |
| 37:f:89:ASP:HB3   | 37:f:93:GLY:H     | 1.86                     | 0.41              |
| 44:p:30:TYR:HA    | 44:p:107:GLN:O    | 2.21                     | 0.41              |
| 46:r:56:ILE:HD11  | 46:r:62:LEU:HD11  | 2.02                     | 0.41              |
| 47:s:244:LEU:HD13 | 47:s:244:LEU:HA   | 1.88                     | 0.41              |
| 47:s:275:ILE:HD13 | 47:s:275:ILE:HA   | 1.85                     | 0.41              |
| 50:v:241:GLN:OE1  | 52:x:32:PRO:HA    | 2.20                     | 0.41              |
| 50:v:241:GLN:NE2  | 52:x:59:TYR:CE2   | 2.89                     | 0.41              |
| 53:y:83:PHE:HA    | 53:y:86:LEU:HD12  | 2.03                     | 0.41              |
| 53:y:502:ILE:HD12 | 53:y:502:ILE:HA   | 1.87                     | 0.41              |
| 53:y:594:LEU:HD22 | 53:y:598:ILE:HD13 | 2.03                     | 0.41              |
| 7:8:235:SER:O     | 7:8:240:GLY:N     | 2.39                     | 0.41              |
| 9:A:14:C:P        | 20:L:190:SER:HG   | 2.44                     | 0.41              |
| 9:A:385:G:H3'     | 10:B:136:LYS:HB2  | 2.03                     | 0.41              |
| 9:A:472:C:O2'     | 9:A:474:G:OP1     | 2.33                     | 0.41              |
| 9:A:1446:A:H5''   | 38:h:58:THR:HG23  | 2.03                     | 0.41              |
| 9:A:1673:U:H5''   | 30:Y:78:VAL:HB    | 2.02                     | 0.41              |
| 13:E:41:PHE:HZ    | 13:E:102:VAL:HG12 | 1.85                     | 0.41              |
| 17:I:28:LEU:HD23  | 17:I:28:LEU:HA    | 1.88                     | 0.41              |
| 28:T:51:THR:HG22  | 28:T:53:ASP:H     | 1.86                     | 0.41              |
| 30:Y:26:LYS:HB2   | 30:Y:26:LYS:HE3   | 1.90                     | 0.41              |
| 30:Y:95:TYR:CE1   | 30:Y:99:TYR:HD2   | 2.38                     | 0.41              |
| 33:b:118:GLU:HB2  | 37:f:120:HIS:H    | 1.84                     | 0.41              |
| 34:c:33:SER:HB3   | 34:c:43:TRP:HE1   | 1.86                     | 0.41              |
| 34:c:232:GLY:HA3  | 34:c:252:THR:HG21 | 2.03                     | 0.41              |
| 45:q:26:LEU:HG    | 45:q:99:GLU:HB2   | 2.03                     | 0.41              |
| 46:r:21:MET:HG3   | 46:r:68:ASN:HB2   | 2.02                     | 0.41              |
| 49:u:260:PHE:HD1  | 49:u:260:PHE:HA   | 1.75                     | 0.41              |
| 49:u:535:GLU:HA   | 49:u:538:LYS:HD2  | 2.03                     | 0.41              |
| 5:6:252:TYR:O     | 5:6:257:GLN:N     | 2.49                     | 0.40              |
| 11:C:52:LEU:HD23  | 11:C:52:LEU:HA    | 1.74                     | 0.40              |
| 21:M:58:MET:HE3   | 21:M:58:MET:HB3   | 1.91                     | 0.40              |
| 22:N:89:LYS:HA    | 22:N:89:LYS:HD3   | 1.86                     | 0.40              |
| 23:O:181:LEU:HA   | 23:O:184:VAL:HG12 | 2.03                     | 0.40              |
| 24:P:30:VAL:N     | 24:P:45:THR:O     | 2.54                     | 0.40              |
| 29:V:66:CYS:HB3   | 29:V:71:ARG:HD3   | 2.04                     | 0.40              |
| 30:Y:146:ARG:HH11 | 30:Y:146:ARG:HA   | 1.86                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 49:u:279:VAL:HG12 | 49:u:295:THR:HG21 | 2.03                     | 0.40              |
| 50:v:344:PHE:CE2  | 50:v:351:ILE:HG22 | 2.55                     | 0.40              |
| 50:v:349:GLN:HE21 | 53:y:833:ALA:HB1  | 1.86                     | 0.40              |
| 52:x:70:ALA:HB2   | 53:y:597:ASN:HB3  | 2.02                     | 0.40              |
| 52:x:412:LYS:HD3  | 52:x:416:GLN:HB3  | 2.02                     | 0.40              |
| 53:y:445:LEU:HA   | 53:y:448:VAL:HG22 | 2.03                     | 0.40              |
| 53:y:508:LEU:HD23 | 53:y:508:LEU:HA   | 1.88                     | 0.40              |
| 53:y:801:SER:HA   | 53:y:842:VAL:HA   | 2.03                     | 0.40              |
| 1:1:512:VAL:HG13  | 1:1:530:VAL:HG13  | 2.03                     | 0.40              |
| 9:A:402:C:OP1     | 26:R:14:THR:OG1   | 2.25                     | 0.40              |
| 9:A:936:G:O2'     | 17:I:105:ASN:HB3  | 2.21                     | 0.40              |
| 9:A:1261:C:OP1    | 9:A:1518:C:N4     | 2.50                     | 0.40              |
| 9:A:1524:G:C8     | 37:f:141:ARG:NH2  | 2.87                     | 0.40              |
| 22:N:34:MET:HE3   | 22:N:34:MET:HB3   | 1.92                     | 0.40              |
| 23:O:128:LYS:HB2  | 23:O:128:LYS:HE2  | 1.89                     | 0.40              |
| 33:b:83:MET:HB3   | 33:b:116:LEU:HD12 | 2.03                     | 0.40              |
| 49:u:80:GLN:HG2   | 49:u:169:ARG:HE   | 1.86                     | 0.40              |
| 49:u:568:ILE:HD13 | 49:u:568:ILE:HA   | 1.89                     | 0.40              |
| 50:v:51:VAL:O     | 50:v:55:MET:N     | 2.50                     | 0.40              |
| 52:x:288:LEU:HB2  | 52:x:317:THR:HG21 | 2.03                     | 0.40              |
| 53:y:57:PHE:HD1   | 53:y:57:PHE:HA    | 1.75                     | 0.40              |
| 53:y:769:PHE:CD2  | 53:y:775:VAL:HG11 | 2.56                     | 0.40              |
| 1:1:472:TRP:HZ3   | 1:1:498:LEU:HD12  | 1.87                     | 0.40              |
| 9:A:1096:G:H2'    | 9:A:1097:G:O4'    | 2.22                     | 0.40              |
| 9:A:1144:A:H2'    | 9:A:1145:A:C8     | 2.56                     | 0.40              |
| 9:A:1443:C:H5'    | 30:Y:13:PHE:CD1   | 2.57                     | 0.40              |
| 9:A:1464:C:O3'    | 21:M:60:ARG:CZ    | 2.69                     | 0.40              |
| 9:A:1520:G:H2'    | 9:A:1520:G:N3     | 2.37                     | 0.40              |
| 9:A:1616:U:O4     | 33:b:40:ARG:NH1   | 2.54                     | 0.40              |
| 11:C:11:ARG:HA    | 11:C:11:ARG:HD2   | 1.81                     | 0.40              |
| 11:C:137:PRO:HG3  | 27:S:209:TYR:CZ   | 2.57                     | 0.40              |
| 11:C:188:ASN:ND2  | 11:C:218:PHE:HB2  | 2.37                     | 0.40              |
| 17:I:111:ALA:HA   | 17:I:114:ARG:HB2  | 2.02                     | 0.40              |
| 21:M:19:LYS:CE    | 31:Z:213:PRO:HD3  | 2.52                     | 0.40              |
| 26:R:154:LYS:HD3  | 26:R:154:LYS:HA   | 1.86                     | 0.40              |
| 27:S:56:ASN:HA    | 27:S:62:PRO:HA    | 2.02                     | 0.40              |
| 29:V:68:ILE:HD12  | 29:V:68:ILE:HA    | 1.94                     | 0.40              |
| 33:b:85:ILE:HG21  | 33:b:111:MET:HG3  | 2.02                     | 0.40              |
| 47:s:216:LYS:HG2  | 47:s:257:VAL:HG13 | 2.02                     | 0.40              |
| 5:6:17:GLU:HA     | 5:6:20:ALA:HB3    | 2.03                     | 0.40              |
| 9:A:912:C:C2      | 9:A:914:U:H1'     | 2.56                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:A:1548:G:N1     | 9:A:1586:U:O4     | 2.54                     | 0.40              |
| 9:A:1825:A:H62    | 45:q:61:ILE:HG21  | 1.86                     | 0.40              |
| 11:C:128:LYS:HG2  | 11:C:129:ILE:N    | 2.37                     | 0.40              |
| 17:I:40:LEU:HD23  | 17:I:40:LEU:HA    | 1.94                     | 0.40              |
| 18:J:11:LEU:HD12  | 18:J:74:VAL:HG12  | 2.04                     | 0.40              |
| 24:P:151:LEU:HA   | 24:P:151:LEU:HD23 | 1.86                     | 0.40              |
| 25:Q:26:CYS:O     | 25:Q:27:ALA:HB3   | 2.22                     | 0.40              |
| 29:V:103:LEU:HD23 | 29:V:103:LEU:HA   | 1.83                     | 0.40              |
| 32:a:1:MET:HE3    | 32:a:1:MET:HB2    | 1.73                     | 0.40              |
| 39:i:21:CYS:SG    | 39:i:39:CYS:HB3   | 2.62                     | 0.40              |
| 40:k:142:GLY:C    | 40:k:144:CYS:H    | 2.29                     | 0.40              |
| 41:m:124:ILE:HA   | 41:m:127:TYR:HB2  | 2.02                     | 0.40              |
| 49:u:490:THR:OG1  | 49:u:491:LEU:N    | 2.53                     | 0.40              |
| 53:y:369:GLY:HA3  | 53:y:425:LEU:HD11 | 2.03                     | 0.40              |
| 9:A:70:G:H21      | 9:A:79:A:H62      | 1.70                     | 0.40              |
| 9:A:436:G:OP2     | 9:A:471:G:O2'     | 2.35                     | 0.40              |
| 9:A:857:U:H2'     | 9:A:858:A:C8      | 2.57                     | 0.40              |
| 9:A:972:A:N6      | 24:P:55:ARG:HH22  | 2.19                     | 0.40              |
| 9:A:1058:A:H2'    | 9:A:1059:G:C8     | 2.57                     | 0.40              |
| 9:A:1534:C:OP1    | 29:V:163:PHE:HA   | 2.22                     | 0.40              |
| 9:A:1750:C:N3     | 9:A:1751:C:N4     | 2.69                     | 0.40              |
| 11:C:36:HIS:CG    | 11:C:85:GLY:HA3   | 2.56                     | 0.40              |
| 11:C:122:LYS:HD2  | 11:C:164:LEU:HD21 | 2.04                     | 0.40              |
| 12:D:87:LEU:HD12  | 12:D:87:LEU:HA    | 1.91                     | 0.40              |
| 20:L:176:LYS:HD2  | 20:L:177:PRO:HD2  | 2.03                     | 0.40              |
| 26:R:3:ILE:H      | 26:R:3:ILE:HD12   | 1.86                     | 0.40              |
| 26:R:124:LYS:HA   | 26:R:124:LYS:HD2  | 1.67                     | 0.40              |
| 27:S:44:GLU:HG3   | 27:S:45:TRP:CD1   | 2.54                     | 0.40              |
| 33:b:67:ALA:HA    | 33:b:68:PRO:HD3   | 1.97                     | 0.40              |
| 34:c:240:CYS:SG   | 34:c:291:TRP:HD1  | 2.45                     | 0.40              |
| 38:h:26:SER:HB3   | 38:h:32:LEU:HD22  | 2.03                     | 0.40              |
| 41:m:35:ILE:HD13  | 41:m:61:TYR:CZ    | 2.57                     | 0.40              |
| 50:v:381:ASP:OD1  | 50:v:381:ASP:N    | 2.52                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed      | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|------------|----------|----------|-------------|-----|
| 1   | 1     | 420/813 (52%) | 394 (94%)  | 20 (5%)  | 6 (1%)   | 9           | 39  |
| 2   | 3     | 209/218 (96%) | 205 (98%)  | 4 (2%)   | 0        | 100         | 100 |
| 3   | 4     | 251/357 (70%) | 230 (92%)  | 18 (7%)  | 3 (1%)   | 10          | 43  |
| 4   | 5     | 307/564 (54%) | 299 (97%)  | 8 (3%)   | 0        | 100         | 100 |
| 5   | 6     | 348/374 (93%) | 320 (92%)  | 28 (8%)  | 0        | 100         | 100 |
| 7   | 8     | 313/352 (89%) | 276 (88%)  | 36 (12%) | 1 (0%)   | 36          | 72  |
| 8   | 9     | 22/25 (88%)   | 22 (100%)  | 0        | 0        | 100         | 100 |
| 10  | B     | 138/158 (87%) | 132 (96%)  | 6 (4%)   | 0        | 100         | 100 |
| 11  | C     | 254/263 (97%) | 246 (97%)  | 7 (3%)   | 1 (0%)   | 30          | 67  |
| 12  | D     | 175/194 (90%) | 175 (100%) | 0        | 0        | 100         | 100 |
| 13  | E     | 138/143 (96%) | 136 (99%)  | 1 (1%)   | 1 (1%)   | 18          | 55  |
| 14  | F     | 38/59 (64%)   | 37 (97%)   | 1 (3%)   | 0        | 100         | 100 |
| 15  | G     | 171/194 (88%) | 163 (95%)  | 8 (5%)   | 0        | 100         | 100 |
| 16  | H     | 79/84 (94%)   | 77 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 17  | I     | 148/151 (98%) | 144 (97%)  | 4 (3%)   | 0        | 100         | 100 |
| 18  | J     | 127/130 (98%) | 123 (97%)  | 4 (3%)   | 0        | 100         | 100 |
| 19  | K     | 79/83 (95%)   | 77 (98%)   | 2 (2%)   | 0        | 100         | 100 |
| 20  | L     | 218/293 (74%) | 210 (96%)  | 8 (4%)   | 0        | 100         | 100 |
| 21  | M     | 129/135 (96%) | 123 (95%)  | 5 (4%)   | 1 (1%)   | 16          | 53  |
| 22  | N     | 205/295 (70%) | 196 (96%)  | 9 (4%)   | 0        | 100         | 100 |
| 23  | O     | 209/264 (79%) | 198 (95%)  | 10 (5%)  | 1 (0%)   | 24          | 63  |
| 24  | P     | 131/151 (87%) | 120 (92%)  | 11 (8%)  | 0        | 100         | 100 |
| 25  | Q     | 97/115 (84%)  | 94 (97%)   | 2 (2%)   | 1 (1%)   | 12          | 47  |
| 26  | R     | 194/208 (93%) | 192 (99%)  | 2 (1%)   | 0        | 100         | 100 |
| 27  | S     | 228/249 (92%) | 225 (99%)  | 3 (1%)   | 0        | 100         | 100 |

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| Mol | Chain | Analysed         | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|------------------|------------|----------|----------|-------------|-----|
| 28  | T     | 123/133 (92%)    | 123 (100%) | 0        | 0        | 100         | 100 |
| 29  | V     | 180/204 (88%)    | 173 (96%)  | 6 (3%)   | 1 (1%)   | 21          | 59  |
| 30  | Y     | 139/146 (95%)    | 137 (99%)  | 2 (1%)   | 0        | 100         | 100 |
| 31  | Z     | 225/243 (93%)    | 221 (98%)  | 4 (2%)   | 0        | 100         | 100 |
| 32  | a     | 97/165 (59%)     | 94 (97%)   | 3 (3%)   | 0        | 100         | 100 |
| 33  | b     | 108/145 (74%)    | 104 (96%)  | 4 (4%)   | 0        | 100         | 100 |
| 34  | c     | 311/317 (98%)    | 304 (98%)  | 7 (2%)   | 0        | 100         | 100 |
| 35  | d     | 140/145 (97%)    | 135 (96%)  | 5 (4%)   | 0        | 100         | 100 |
| 36  | e     | 64/125 (51%)     | 62 (97%)   | 2 (3%)   | 0        | 100         | 100 |
| 37  | f     | 140/152 (92%)    | 136 (97%)  | 4 (3%)   | 0        | 100         | 100 |
| 38  | h     | 101/119 (85%)    | 98 (97%)   | 3 (3%)   | 0        | 100         | 100 |
| 39  | i     | 48/56 (86%)      | 45 (94%)   | 2 (4%)   | 1 (2%)   | 5           | 29  |
| 40  | k     | 49/156 (31%)     | 46 (94%)   | 2 (4%)   | 1 (2%)   | 6           | 31  |
| 41  | m     | 120/132 (91%)    | 114 (95%)  | 5 (4%)   | 1 (1%)   | 16          | 53  |
| 42  | n     | 61/69 (88%)      | 59 (97%)   | 2 (3%)   | 0        | 100         | 100 |
| 43  | o     | 75/320 (23%)     | 74 (99%)   | 1 (1%)   | 0        | 100         | 100 |
| 44  | p     | 83/113 (74%)     | 81 (98%)   | 1 (1%)   | 1 (1%)   | 10          | 43  |
| 45  | q     | 86/144 (60%)     | 75 (87%)   | 9 (10%)  | 2 (2%)   | 5           | 28  |
| 46  | r     | 273/315 (87%)    | 249 (91%)  | 23 (8%)  | 1 (0%)   | 30          | 67  |
| 47  | s     | 136/333 (41%)    | 120 (88%)  | 15 (11%) | 1 (1%)   | 18          | 55  |
| 48  | t     | 346/472 (73%)    | 329 (95%)  | 11 (3%)  | 6 (2%)   | 7           | 35  |
| 49  | u     | 705/1382 (51%)   | 676 (96%)  | 28 (4%)  | 1 (0%)   | 48          | 83  |
| 50  | v     | 380/445 (85%)    | 349 (92%)  | 31 (8%)  | 0        | 100         | 100 |
| 52  | x     | 415/548 (76%)    | 385 (93%)  | 30 (7%)  | 0        | 100         | 100 |
| 53  | y     | 691/913 (76%)    | 661 (96%)  | 29 (4%)  | 1 (0%)   | 48          | 83  |
| All | All   | 9724/13164 (74%) | 9264 (95%) | 428 (4%) | 32 (0%)  | 37          | 72  |

All (32) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1     | 282 | PRO  |
| 1   | 1     | 427 | PRO  |
| 1   | 1     | 648 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | 4     | 264 | GLY  |
| 23  | O     | 117 | TRP  |
| 29  | V     | 203 | ASN  |
| 39  | i     | 8   | TRP  |
| 41  | m     | 92  | CYS  |
| 48  | t     | 167 | GLN  |
| 48  | t     | 168 | PRO  |
| 48  | t     | 224 | ILE  |
| 1   | 1     | 647 | ASN  |
| 7   | 8     | 154 | PRO  |
| 40  | k     | 102 | VAL  |
| 44  | p     | 40  | GLY  |
| 45  | q     | 86  | ASP  |
| 46  | r     | 195 | ILE  |
| 48  | t     | 247 | PRO  |
| 48  | t     | 248 | ARG  |
| 1   | 1     | 286 | PRO  |
| 1   | 1     | 499 | PRO  |
| 3   | 4     | 263 | ILE  |
| 11  | C     | 24  | THR  |
| 45  | q     | 87  | ASN  |
| 47  | s     | 190 | LYS  |
| 48  | t     | 222 | ILE  |
| 53  | y     | 849 | PRO  |
| 3   | 4     | 320 | PRO  |
| 13  | E     | 137 | LYS  |
| 21  | M     | 92  | ASP  |
| 25  | Q     | 96  | THR  |
| 49  | u     | 539 | PRO  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed     | Rotameric | Outliers | Percentiles |
|-----|-------|--------------|-----------|----------|-------------|
| 1   | 1     | 97/701 (14%) | 95 (98%)  | 2 (2%)   | 47 65       |
| 5   | 6     | 49/335 (15%) | 47 (96%)  | 2 (4%)   | 27 49       |

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| Mol | Chain | Analysed      | Rotameric | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|-------------|-----|
| 8   | 9     | 23/24 (96%)   | 22 (96%)  | 1 (4%)   | 26          | 48  |
| 10  | B     | 129/142 (91%) | 115 (89%) | 14 (11%) | 6           | 21  |
| 11  | C     | 220/225 (98%) | 188 (86%) | 32 (14%) | 3           | 14  |
| 12  | D     | 158/168 (94%) | 155 (98%) | 3 (2%)   | 50          | 66  |
| 13  | E     | 112/115 (97%) | 109 (97%) | 3 (3%)   | 39          | 60  |
| 14  | F     | 33/48 (69%)   | 25 (76%)  | 8 (24%)  | 1           | 5   |
| 15  | G     | 159/174 (91%) | 155 (98%) | 4 (2%)   | 42          | 62  |
| 16  | H     | 73/76 (96%)   | 72 (99%)  | 1 (1%)   | 59          | 72  |
| 17  | I     | 130/131 (99%) | 129 (99%) | 1 (1%)   | 73          | 78  |
| 18  | J     | 112/113 (99%) | 108 (96%) | 4 (4%)   | 31          | 52  |
| 19  | K     | 65/67 (97%)   | 65 (100%) | 0        | 100         | 100 |
| 20  | L     | 186/225 (83%) | 181 (97%) | 5 (3%)   | 39          | 60  |
| 21  | M     | 119/122 (98%) | 106 (89%) | 13 (11%) | 6           | 21  |
| 22  | N     | 173/243 (71%) | 172 (99%) | 1 (1%)   | 78          | 81  |
| 23  | O     | 192/231 (83%) | 189 (98%) | 3 (2%)   | 55          | 69  |
| 24  | P     | 104/119 (87%) | 98 (94%)  | 6 (6%)   | 18          | 40  |
| 25  | Q     | 86/98 (88%)   | 83 (96%)  | 3 (4%)   | 32          | 54  |
| 26  | R     | 172/180 (96%) | 165 (96%) | 7 (4%)   | 27          | 49  |
| 27  | S     | 200/218 (92%) | 194 (97%) | 6 (3%)   | 36          | 57  |
| 28  | T     | 107/115 (93%) | 101 (94%) | 6 (6%)   | 19          | 41  |
| 29  | V     | 156/170 (92%) | 152 (97%) | 4 (3%)   | 40          | 61  |
| 30  | Y     | 117/121 (97%) | 106 (91%) | 11 (9%)  | 8           | 26  |
| 31  | Z     | 190/202 (94%) | 178 (94%) | 12 (6%)  | 16          | 38  |
| 32  | a     | 90/136 (66%)  | 83 (92%)  | 7 (8%)   | 11          | 32  |
| 33  | b     | 100/130 (77%) | 98 (98%)  | 2 (2%)   | 48          | 66  |
| 34  | c     | 272/275 (99%) | 262 (96%) | 10 (4%)  | 30          | 51  |
| 35  | d     | 112/115 (97%) | 106 (95%) | 6 (5%)   | 20          | 42  |
| 36  | e     | 58/103 (56%)  | 56 (97%)  | 2 (3%)   | 32          | 55  |
| 37  | f     | 123/132 (93%) | 119 (97%) | 4 (3%)   | 33          | 55  |
| 38  | h     | 94/107 (88%)  | 94 (100%) | 0        | 100         | 100 |
| 39  | i     | 44/49 (90%)   | 35 (80%)  | 9 (20%)  | 1           | 7   |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 40  | k     | 47/140 (34%)    | 31 (66%)   | 16 (34%) | 0           | 2  |
| 41  | m     | 104/108 (96%)   | 89 (86%)   | 15 (14%) | 3           | 14 |
| 42  | n     | 56/62 (90%)     | 55 (98%)   | 1 (2%)   | 51          | 67 |
| 43  | o     | 64/277 (23%)    | 58 (91%)   | 6 (9%)   | 8           | 26 |
| 44  | p     | 74/96 (77%)     | 59 (80%)   | 15 (20%) | 1           | 8  |
| 45  | q     | 75/123 (61%)    | 52 (69%)   | 23 (31%) | 0           | 2  |
| 46  | r     | 247/280 (88%)   | 225 (91%)  | 22 (9%)  | 9           | 28 |
| 47  | s     | 128/304 (42%)   | 116 (91%)  | 12 (9%)  | 8           | 26 |
| 49  | u     | 528/1259 (42%)  | 517 (98%)  | 11 (2%)  | 47          | 65 |
| 50  | v     | 206/406 (51%)   | 197 (96%)  | 9 (4%)   | 25          | 47 |
| 52  | x     | 206/494 (42%)   | 201 (98%)  | 5 (2%)   | 43          | 63 |
| 53  | y     | 564/811 (70%)   | 555 (98%)  | 9 (2%)   | 55          | 69 |
| All | All   | 6354/9770 (65%) | 6018 (95%) | 336 (5%) | 22          | 42 |

All (336) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 1     | 554 | VAL  |
| 1   | 1     | 566 | ILE  |
| 5   | 6     | 326 | ASP  |
| 5   | 6     | 333 | VAL  |
| 8   | 9     | 23  | ARG  |
| 10  | B     | 4   | ILE  |
| 10  | B     | 11  | GLN  |
| 10  | B     | 15  | THR  |
| 10  | B     | 33  | LEU  |
| 10  | B     | 35  | ARG  |
| 10  | B     | 37  | TYR  |
| 10  | B     | 46  | THR  |
| 10  | B     | 65  | ASN  |
| 10  | B     | 74  | SER  |
| 10  | B     | 104 | LYS  |
| 10  | B     | 111 | VAL  |
| 10  | B     | 135 | SER  |
| 10  | B     | 138 | VAL  |
| 10  | B     | 151 | THR  |
| 11  | C     | 17  | HIS  |
| 11  | C     | 21  | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11  | C     | 26  | VAL  |
| 11  | C     | 45  | ILE  |
| 11  | C     | 52  | LEU  |
| 11  | C     | 54  | TYR  |
| 11  | C     | 56  | LEU  |
| 11  | C     | 57  | THR  |
| 11  | C     | 79  | ASP  |
| 11  | C     | 87  | MET  |
| 11  | C     | 92  | ILE  |
| 11  | C     | 102 | ILE  |
| 11  | C     | 105 | THR  |
| 11  | C     | 109 | PHE  |
| 11  | C     | 111 | VAL  |
| 11  | C     | 113 | ARG  |
| 11  | C     | 122 | LYS  |
| 11  | C     | 129 | ILE  |
| 11  | C     | 154 | ILE  |
| 11  | C     | 166 | THR  |
| 11  | C     | 170 | THR  |
| 11  | C     | 173 | ILE  |
| 11  | C     | 194 | VAL  |
| 11  | C     | 196 | THR  |
| 11  | C     | 210 | VAL  |
| 11  | C     | 216 | ASN  |
| 11  | C     | 220 | THR  |
| 11  | C     | 222 | LEU  |
| 11  | C     | 225 | ILE  |
| 11  | C     | 236 | ILE  |
| 11  | C     | 240 | ARG  |
| 11  | C     | 248 | ILE  |
| 12  | D     | 3   | VAL  |
| 12  | D     | 154 | GLN  |
| 12  | D     | 155 | LYS  |
| 13  | E     | 125 | VAL  |
| 13  | E     | 139 | GLU  |
| 13  | E     | 140 | ARG  |
| 14  | F     | 80  | LEU  |
| 14  | F     | 82  | ARG  |
| 14  | F     | 90  | THR  |
| 14  | F     | 93  | VAL  |
| 14  | F     | 95  | LYS  |
| 14  | F     | 96  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 14  | F     | 99  | LYS  |
| 14  | F     | 103 | THR  |
| 15  | G     | 98  | ARG  |
| 15  | G     | 100 | ILE  |
| 15  | G     | 121 | THR  |
| 15  | G     | 123 | THR  |
| 16  | H     | 25  | VAL  |
| 17  | I     | 20  | ARG  |
| 18  | J     | 2   | VAL  |
| 18  | J     | 30  | CYS  |
| 18  | J     | 54  | ASP  |
| 18  | J     | 80  | ASP  |
| 20  | L     | 115 | GLN  |
| 20  | L     | 116 | THR  |
| 20  | L     | 120 | GLN  |
| 20  | L     | 227 | ARG  |
| 20  | L     | 230 | THR  |
| 21  | M     | 16  | ILE  |
| 21  | M     | 17  | ILE  |
| 21  | M     | 47  | ARG  |
| 21  | M     | 61  | ILE  |
| 21  | M     | 66  | VAL  |
| 21  | M     | 69  | ILE  |
| 21  | M     | 72  | LYS  |
| 21  | M     | 75  | GLU  |
| 21  | M     | 79  | GLU  |
| 21  | M     | 81  | ARG  |
| 21  | M     | 82  | ASP  |
| 21  | M     | 85  | VAL  |
| 21  | M     | 128 | PHE  |
| 22  | N     | 33  | GLN  |
| 23  | O     | 48  | LEU  |
| 23  | O     | 111 | CYS  |
| 23  | O     | 210 | VAL  |
| 24  | P     | 21  | VAL  |
| 24  | P     | 52  | THR  |
| 24  | P     | 103 | ASN  |
| 24  | P     | 143 | LYS  |
| 24  | P     | 150 | ARG  |
| 24  | P     | 151 | LEU  |
| 25  | Q     | 12  | LYS  |
| 25  | Q     | 15  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 25  | Q     | 86  | ASN  |
| 26  | R     | 62  | VAL  |
| 26  | R     | 72  | CYS  |
| 26  | R     | 119 | LEU  |
| 26  | R     | 136 | ILE  |
| 26  | R     | 142 | SER  |
| 26  | R     | 143 | LYS  |
| 26  | R     | 145 | ILE  |
| 27  | S     | 32  | MET  |
| 27  | S     | 44  | GLU  |
| 27  | S     | 101 | ILE  |
| 27  | S     | 153 | VAL  |
| 27  | S     | 158 | VAL  |
| 27  | S     | 181 | THR  |
| 28  | T     | 9   | THR  |
| 28  | T     | 50  | THR  |
| 28  | T     | 80  | ASP  |
| 28  | T     | 96  | LEU  |
| 28  | T     | 100 | LYS  |
| 28  | T     | 102 | THR  |
| 29  | V     | 41  | VAL  |
| 29  | V     | 119 | SER  |
| 29  | V     | 193 | LYS  |
| 29  | V     | 195 | GLU  |
| 30  | Y     | 11  | GLN  |
| 30  | Y     | 20  | THR  |
| 30  | Y     | 25  | CYS  |
| 30  | Y     | 43  | GLU  |
| 30  | Y     | 47  | LEU  |
| 30  | Y     | 57  | LEU  |
| 30  | Y     | 67  | ASP  |
| 30  | Y     | 81  | ILE  |
| 30  | Y     | 100 | VAL  |
| 30  | Y     | 123 | ASP  |
| 30  | Y     | 143 | LYS  |
| 31  | Z     | 42  | THR  |
| 31  | Z     | 44  | THR  |
| 31  | Z     | 66  | ILE  |
| 31  | Z     | 84  | VAL  |
| 31  | Z     | 86  | LEU  |
| 31  | Z     | 139 | SER  |
| 31  | Z     | 149 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 31  | Z     | 156 | LEU  |
| 31  | Z     | 162 | ASP  |
| 31  | Z     | 163 | PRO  |
| 31  | Z     | 179 | GLN  |
| 31  | Z     | 209 | SER  |
| 32  | a     | 29  | MET  |
| 32  | a     | 40  | VAL  |
| 32  | a     | 53  | LYS  |
| 32  | a     | 66  | HIS  |
| 32  | a     | 67  | PHE  |
| 32  | a     | 74  | GLU  |
| 32  | a     | 93  | THR  |
| 33  | b     | 88  | GLU  |
| 33  | b     | 121 | ILE  |
| 34  | c     | 107 | ASP  |
| 34  | c     | 113 | PHE  |
| 34  | c     | 116 | ASP  |
| 34  | c     | 134 | THR  |
| 34  | c     | 142 | VAL  |
| 34  | c     | 199 | THR  |
| 34  | c     | 227 | LEU  |
| 34  | c     | 265 | ILE  |
| 34  | c     | 275 | ILE  |
| 34  | c     | 277 | THR  |
| 35  | d     | 34  | VAL  |
| 35  | d     | 63  | HIS  |
| 35  | d     | 66  | LEU  |
| 35  | d     | 96  | SER  |
| 35  | d     | 123 | LEU  |
| 35  | d     | 125 | PRO  |
| 36  | e     | 51  | ASP  |
| 36  | e     | 58  | LEU  |
| 37  | f     | 25  | LYS  |
| 37  | f     | 31  | THR  |
| 37  | f     | 60  | THR  |
| 37  | f     | 83  | PHE  |
| 39  | i     | 9   | SER  |
| 39  | i     | 12  | ARG  |
| 39  | i     | 16  | GLN  |
| 39  | i     | 19  | ARG  |
| 39  | i     | 30  | LEU  |
| 39  | i     | 31  | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 39  | i     | 36  | LEU  |
| 39  | i     | 39  | CYS  |
| 39  | i     | 40  | ARG  |
| 40  | k     | 94  | LYS  |
| 40  | k     | 96  | LYS  |
| 40  | k     | 100 | LEU  |
| 40  | k     | 102 | VAL  |
| 40  | k     | 104 | LYS  |
| 40  | k     | 106 | TYR  |
| 40  | k     | 114 | ILE  |
| 40  | k     | 119 | ARG  |
| 40  | k     | 125 | GLU  |
| 40  | k     | 126 | CYS  |
| 40  | k     | 132 | MET  |
| 40  | k     | 137 | ASP  |
| 40  | k     | 138 | ARG  |
| 40  | k     | 140 | TYR  |
| 40  | k     | 141 | CYS  |
| 40  | k     | 143 | LYS  |
| 41  | m     | 12  | MET  |
| 41  | m     | 51  | VAL  |
| 41  | m     | 52  | LEU  |
| 41  | m     | 58  | GLU  |
| 41  | m     | 62  | VAL  |
| 41  | m     | 66  | GLU  |
| 41  | m     | 74  | ILE  |
| 41  | m     | 77  | ILE  |
| 41  | m     | 91  | LEU  |
| 41  | m     | 96  | ARG  |
| 41  | m     | 103 | VAL  |
| 41  | m     | 109 | VAL  |
| 41  | m     | 112 | LYS  |
| 41  | m     | 124 | ILE  |
| 41  | m     | 132 | LYS  |
| 42  | n     | 46  | VAL  |
| 43  | o     | 240 | THR  |
| 43  | o     | 286 | SER  |
| 43  | o     | 297 | ILE  |
| 43  | o     | 305 | TYR  |
| 43  | o     | 308 | LEU  |
| 43  | o     | 313 | GLU  |
| 44  | p     | 33  | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 44  | p     | 43  | THR  |
| 44  | p     | 48  | GLN  |
| 44  | p     | 50  | ILE  |
| 44  | p     | 58  | LYS  |
| 44  | p     | 59  | LEU  |
| 44  | p     | 60  | VAL  |
| 44  | p     | 65  | LYS  |
| 44  | p     | 85  | LEU  |
| 44  | p     | 97  | LEU  |
| 44  | p     | 98  | VAL  |
| 44  | p     | 102 | LEU  |
| 44  | p     | 108 | LEU  |
| 44  | p     | 110 | VAL  |
| 44  | p     | 113 | PHE  |
| 45  | q     | 22  | GLU  |
| 45  | q     | 24  | ARG  |
| 45  | q     | 25  | GLU  |
| 45  | q     | 26  | LEU  |
| 45  | q     | 28  | PHE  |
| 45  | q     | 33  | GLN  |
| 45  | q     | 35  | TYR  |
| 45  | q     | 38  | VAL  |
| 45  | q     | 39  | ILE  |
| 45  | q     | 47  | LEU  |
| 45  | q     | 51  | CYS  |
| 45  | q     | 55  | VAL  |
| 45  | q     | 61  | ILE  |
| 45  | q     | 62  | ARG  |
| 45  | q     | 64  | LYS  |
| 45  | q     | 73  | THR  |
| 45  | q     | 81  | LEU  |
| 45  | q     | 83  | ASP  |
| 45  | q     | 86  | ASP  |
| 45  | q     | 99  | GLU  |
| 45  | q     | 103 | LEU  |
| 45  | q     | 108 | GLU  |
| 45  | q     | 109 | LEU  |
| 46  | r     | 20  | VAL  |
| 46  | r     | 33  | TYR  |
| 46  | r     | 34  | VAL  |
| 46  | r     | 47  | LEU  |
| 46  | r     | 48  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 46  | r     | 56  | ILE  |
| 46  | r     | 72  | VAL  |
| 46  | r     | 73  | VAL  |
| 46  | r     | 76  | VAL  |
| 46  | r     | 78  | LYS  |
| 46  | r     | 88  | ARG  |
| 46  | r     | 89  | ARG  |
| 46  | r     | 121 | TYR  |
| 46  | r     | 179 | ASN  |
| 46  | r     | 194 | ASP  |
| 46  | r     | 195 | ILE  |
| 46  | r     | 229 | LEU  |
| 46  | r     | 240 | THR  |
| 46  | r     | 248 | LEU  |
| 46  | r     | 271 | VAL  |
| 46  | r     | 277 | VAL  |
| 46  | r     | 278 | VAL  |
| 47  | s     | 187 | MET  |
| 47  | s     | 195 | VAL  |
| 47  | s     | 200 | ARG  |
| 47  | s     | 220 | VAL  |
| 47  | s     | 228 | LEU  |
| 47  | s     | 234 | LYS  |
| 47  | s     | 243 | GLU  |
| 47  | s     | 244 | LEU  |
| 47  | s     | 275 | ILE  |
| 47  | s     | 279 | VAL  |
| 47  | s     | 290 | ILE  |
| 47  | s     | 304 | THR  |
| 49  | u     | 109 | GLN  |
| 49  | u     | 331 | ILE  |
| 49  | u     | 337 | ASP  |
| 49  | u     | 340 | ARG  |
| 49  | u     | 448 | GLN  |
| 49  | u     | 459 | VAL  |
| 49  | u     | 558 | LEU  |
| 49  | u     | 562 | ARG  |
| 49  | u     | 563 | LYS  |
| 49  | u     | 568 | ILE  |
| 49  | u     | 572 | ARG  |
| 50  | v     | 203 | SER  |
| 50  | v     | 205 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 50  | v     | 226 | PRO  |
| 50  | v     | 237 | LEU  |
| 50  | v     | 243 | LEU  |
| 50  | v     | 246 | ILE  |
| 50  | v     | 273 | VAL  |
| 50  | v     | 377 | ASN  |
| 50  | v     | 392 | VAL  |
| 52  | x     | 368 | ASP  |
| 52  | x     | 385 | ASN  |
| 52  | x     | 466 | LEU  |
| 52  | x     | 471 | PHE  |
| 52  | x     | 475 | GLU  |
| 53  | y     | 67  | ILE  |
| 53  | y     | 77  | THR  |
| 53  | y     | 102 | VAL  |
| 53  | y     | 116 | TYR  |
| 53  | y     | 140 | THR  |
| 53  | y     | 143 | GLN  |
| 53  | y     | 779 | LEU  |
| 53  | y     | 841 | THR  |
| 53  | y     | 854 | ASN  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10  | B     | 5   | GLN  |
| 10  | B     | 65  | ASN  |
| 10  | B     | 83  | GLN  |
| 10  | B     | 112 | HIS  |
| 11  | C     | 67  | GLN  |
| 11  | C     | 98  | ASN  |
| 13  | E     | 23  | HIS  |
| 17  | I     | 36  | GLN  |
| 18  | J     | 70  | ASN  |
| 21  | M     | 56  | HIS  |
| 21  | M     | 118 | GLN  |
| 22  | N     | 193 | HIS  |
| 25  | Q     | 8   | ASN  |
| 25  | Q     | 43  | ASN  |
| 25  | Q     | 86  | ASN  |
| 26  | R     | 167 | GLN  |
| 27  | S     | 146 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 28  | T     | 19  | GLN  |
| 30  | Y     | 24  | HIS  |
| 31  | Z     | 56  | GLN  |
| 31  | Z     | 207 | HIS  |
| 32  | a     | 39  | ASN  |
| 32  | a     | 44  | HIS  |
| 32  | a     | 66  | HIS  |
| 33  | b     | 32  | GLN  |
| 35  | d     | 117 | GLN  |
| 37  | f     | 73  | ASN  |
| 38  | h     | 85  | HIS  |
| 40  | k     | 139 | HIS  |
| 41  | m     | 46  | GLN  |
| 43  | o     | 311 | ASN  |
| 44  | p     | 32  | HIS  |
| 46  | r     | 181 | ASN  |
| 47  | s     | 221 | ASN  |
| 49  | u     | 6   | GLN  |
| 49  | u     | 44  | GLN  |
| 49  | u     | 79  | GLN  |
| 49  | u     | 200 | ASN  |
| 49  | u     | 212 | HIS  |
| 49  | u     | 219 | ASN  |
| 49  | u     | 221 | ASN  |
| 49  | u     | 270 | GLN  |
| 49  | u     | 288 | ASN  |
| 49  | u     | 392 | ASN  |
| 49  | u     | 448 | GLN  |
| 49  | u     | 512 | GLN  |
| 49  | u     | 566 | GLN  |
| 50  | v     | 402 | GLN  |
| 52  | x     | 24  | GLN  |
| 52  | x     | 81  | GLN  |
| 52  | x     | 326 | GLN  |
| 53  | y     | 118 | ASN  |
| 53  | y     | 364 | ASN  |
| 53  | y     | 433 | ASN  |
| 53  | y     | 460 | GLN  |
| 53  | y     | 467 | GLN  |
| 53  | y     | 520 | GLN  |
| 53  | y     | 670 | GLN  |
| 53  | y     | 701 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 53  | y     | 717 | GLN  |
| 53  | y     | 852 | GLN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 51  | w     | 74/75 (98%)     | 41 (55%)          | 0               |
| 6   | 7     | 19/20 (95%)     | 15 (78%)          | 0               |
| 9   | A     | 1710/1869 (91%) | 445 (26%)         | 52 (3%)         |
| All | All   | 1803/1964 (91%) | 501 (27%)         | 52 (2%)         |

All (501) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | 7     | 10  | A    |
| 6   | 7     | 11  | A    |
| 6   | 7     | 12  | A    |
| 6   | 7     | 13  | A    |
| 6   | 7     | 14  | A    |
| 6   | 7     | 15  | A    |
| 6   | 7     | 16  | A    |
| 6   | 7     | 18  | A    |
| 6   | 7     | 19  | A    |
| 6   | 7     | 20  | A    |
| 6   | 7     | 22  | A    |
| 6   | 7     | 24  | A    |
| 6   | 7     | 25  | A    |
| 6   | 7     | 26  | A    |
| 6   | 7     | 28  | A    |
| 9   | A     | 2   | A    |
| 9   | A     | 4   | C    |
| 9   | A     | 10  | G    |
| 9   | A     | 11  | A    |
| 9   | A     | 12  | U    |
| 9   | A     | 17  | C    |
| 9   | A     | 23  | G    |
| 9   | A     | 33  | G    |
| 9   | A     | 41  | G    |
| 9   | A     | 42  | A    |
| 9   | A     | 44  | U    |
| 9   | A     | 46  | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9   | A     | 56  | G    |
| 9   | A     | 58  | C    |
| 9   | A     | 59  | U    |
| 9   | A     | 62  | G    |
| 9   | A     | 64  | A    |
| 9   | A     | 65  | C    |
| 9   | A     | 67  | C    |
| 9   | A     | 68  | A    |
| 9   | A     | 72  | C    |
| 9   | A     | 73  | C    |
| 9   | A     | 74  | G    |
| 9   | A     | 78  | C    |
| 9   | A     | 82  | G    |
| 9   | A     | 103 | A    |
| 9   | A     | 110 | U    |
| 9   | A     | 114 | G    |
| 9   | A     | 115 | U    |
| 9   | A     | 126 | G    |
| 9   | A     | 129 | C    |
| 9   | A     | 130 | G    |
| 9   | A     | 140 | U    |
| 9   | A     | 142 | C    |
| 9   | A     | 143 | U    |
| 9   | A     | 147 | A    |
| 9   | A     | 155 | G    |
| 9   | A     | 158 | A    |
| 9   | A     | 160 | U    |
| 9   | A     | 163 | U    |
| 9   | A     | 168 | C    |
| 9   | A     | 173 | A    |
| 9   | A     | 180 | G    |
| 9   | A     | 182 | C    |
| 9   | A     | 184 | G    |
| 9   | A     | 190 | G    |
| 9   | A     | 196 | C    |
| 9   | A     | 197 | U    |
| 9   | A     | 198 | U    |
| 9   | A     | 199 | C    |
| 9   | A     | 200 | G    |
| 9   | A     | 201 | C    |
| 9   | A     | 202 | G    |
| 9   | A     | 203 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9   | A     | 204 | G    |
| 9   | A     | 206 | G    |
| 9   | A     | 208 | G    |
| 9   | A     | 288 | G    |
| 9   | A     | 291 | G    |
| 9   | A     | 292 | A    |
| 9   | A     | 293 | C    |
| 9   | A     | 294 | U    |
| 9   | A     | 295 | C    |
| 9   | A     | 306 | C    |
| 9   | A     | 307 | G    |
| 9   | A     | 308 | G    |
| 9   | A     | 309 | G    |
| 9   | A     | 314 | U    |
| 9   | A     | 318 | A    |
| 9   | A     | 319 | C    |
| 9   | A     | 320 | G    |
| 9   | A     | 321 | C    |
| 9   | A     | 323 | C    |
| 9   | A     | 324 | C    |
| 9   | A     | 325 | C    |
| 9   | A     | 326 | C    |
| 9   | A     | 327 | G    |
| 9   | A     | 328 | U    |
| 9   | A     | 329 | G    |
| 9   | A     | 332 | G    |
| 9   | A     | 347 | G    |
| 9   | A     | 362 | C    |
| 9   | A     | 363 | A    |
| 9   | A     | 364 | A    |
| 9   | A     | 366 | U    |
| 9   | A     | 367 | U    |
| 9   | A     | 368 | U    |
| 9   | A     | 369 | C    |
| 9   | A     | 370 | G    |
| 9   | A     | 371 | A    |
| 9   | A     | 372 | U    |
| 9   | A     | 373 | G    |
| 9   | A     | 374 | G    |
| 9   | A     | 382 | C    |
| 9   | A     | 385 | G    |
| 9   | A     | 386 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9   | A     | 392 | A    |
| 9   | A     | 393 | U    |
| 9   | A     | 394 | G    |
| 9   | A     | 396 | U    |
| 9   | A     | 397 | G    |
| 9   | A     | 409 | C    |
| 9   | A     | 418 | A    |
| 9   | A     | 421 | G    |
| 9   | A     | 447 | A    |
| 9   | A     | 448 | A    |
| 9   | A     | 449 | A    |
| 9   | A     | 450 | C    |
| 9   | A     | 452 | G    |
| 9   | A     | 465 | A    |
| 9   | A     | 471 | G    |
| 9   | A     | 472 | C    |
| 9   | A     | 473 | A    |
| 9   | A     | 474 | G    |
| 9   | A     | 476 | A    |
| 9   | A     | 482 | G    |
| 9   | A     | 487 | U    |
| 9   | A     | 492 | C    |
| 9   | A     | 496 | C    |
| 9   | A     | 497 | C    |
| 9   | A     | 508 | A    |
| 9   | A     | 512 | A    |
| 9   | A     | 516 | A    |
| 9   | A     | 525 | A    |
| 9   | A     | 533 | A    |
| 9   | A     | 534 | G    |
| 9   | A     | 536 | A    |
| 9   | A     | 537 | C    |
| 9   | A     | 538 | U    |
| 9   | A     | 539 | C    |
| 9   | A     | 540 | U    |
| 9   | A     | 541 | U    |
| 9   | A     | 542 | U    |
| 9   | A     | 543 | C    |
| 9   | A     | 544 | G    |
| 9   | A     | 545 | A    |
| 9   | A     | 546 | G    |
| 9   | A     | 547 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9   | A     | 550 | C    |
| 9   | A     | 553 | U    |
| 9   | A     | 554 | A    |
| 9   | A     | 556 | U    |
| 9   | A     | 557 | U    |
| 9   | A     | 558 | G    |
| 9   | A     | 559 | G    |
| 9   | A     | 563 | G    |
| 9   | A     | 564 | A    |
| 9   | A     | 566 | U    |
| 9   | A     | 568 | C    |
| 9   | A     | 576 | A    |
| 9   | A     | 583 | A    |
| 9   | A     | 589 | G    |
| 9   | A     | 590 | A    |
| 9   | A     | 591 | U    |
| 9   | A     | 598 | G    |
| 9   | A     | 604 | A    |
| 9   | A     | 606 | G    |
| 9   | A     | 607 | U    |
| 9   | A     | 614 | C    |
| 9   | A     | 617 | G    |
| 9   | A     | 624 | C    |
| 9   | A     | 626 | G    |
| 9   | A     | 627 | U    |
| 9   | A     | 628 | A    |
| 9   | A     | 629 | A    |
| 9   | A     | 631 | U    |
| 9   | A     | 643 | A    |
| 9   | A     | 655 | A    |
| 9   | A     | 659 | G    |
| 9   | A     | 660 | C    |
| 9   | A     | 662 | G    |
| 9   | A     | 664 | A    |
| 9   | A     | 668 | A2M  |
| 9   | A     | 669 | A    |
| 9   | A     | 671 | A    |
| 9   | A     | 672 | A    |
| 9   | A     | 673 | G    |
| 9   | A     | 687 | C    |
| 9   | A     | 688 | U    |
| 9   | A     | 689 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 9   | A     | 690 | G    |
| 9   | A     | 693 | A    |
| 9   | A     | 694 | G    |
| 9   | A     | 734 | C    |
| 9   | A     | 736 | C    |
| 9   | A     | 748 | C    |
| 9   | A     | 749 | U    |
| 9   | A     | 751 | G    |
| 9   | A     | 752 | G    |
| 9   | A     | 753 | C    |
| 9   | A     | 790 | C    |
| 9   | A     | 791 | C    |
| 9   | A     | 797 | C    |
| 9   | A     | 798 | G    |
| 9   | A     | 799 | U    |
| 9   | A     | 801 | U    |
| 9   | A     | 810 | A    |
| 9   | A     | 811 | A    |
| 9   | A     | 821 | G    |
| 9   | A     | 822 | PSU  |
| 9   | A     | 827 | A    |
| 9   | A     | 830 | A    |
| 9   | A     | 836 | G    |
| 9   | A     | 837 | A    |
| 9   | A     | 838 | G    |
| 9   | A     | 839 | C    |
| 9   | A     | 840 | C    |
| 9   | A     | 841 | G    |
| 9   | A     | 845 | G    |
| 9   | A     | 869 | A    |
| 9   | A     | 870 | A    |
| 9   | A     | 872 | A    |
| 9   | A     | 873 | G    |
| 9   | A     | 878 | G    |
| 9   | A     | 880 | G    |
| 9   | A     | 886 | A    |
| 9   | A     | 888 | U    |
| 9   | A     | 889 | U    |
| 9   | A     | 890 | U    |
| 9   | A     | 891 | G    |
| 9   | A     | 892 | U    |
| 9   | A     | 894 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 9   | A     | 895  | G    |
| 9   | A     | 896  | U    |
| 9   | A     | 897  | U    |
| 9   | A     | 898  | U    |
| 9   | A     | 899  | U    |
| 9   | A     | 900  | C    |
| 9   | A     | 903  | A    |
| 9   | A     | 909  | G    |
| 9   | A     | 912  | C    |
| 9   | A     | 913  | A    |
| 9   | A     | 920  | A    |
| 9   | A     | 922  | A    |
| 9   | A     | 930  | C    |
| 9   | A     | 933  | G    |
| 9   | A     | 943  | U    |
| 9   | A     | 950  | C    |
| 9   | A     | 963  | A    |
| 9   | A     | 965  | U    |
| 9   | A     | 969  | U    |
| 9   | A     | 970  | G    |
| 9   | A     | 989  | C    |
| 9   | A     | 990  | A    |
| 9   | A     | 992  | A    |
| 9   | A     | 999  | G    |
| 9   | A     | 1002 | U    |
| 9   | A     | 1017 | U    |
| 9   | A     | 1023 | A    |
| 9   | A     | 1061 | U    |
| 9   | A     | 1062 | A    |
| 9   | A     | 1083 | A    |
| 9   | A     | 1085 | C    |
| 9   | A     | 1096 | G    |
| 9   | A     | 1109 | C    |
| 9   | A     | 1112 | U    |
| 9   | A     | 1113 | A    |
| 9   | A     | 1114 | U    |
| 9   | A     | 1115 | U    |
| 9   | A     | 1117 | C    |
| 9   | A     | 1120 | U    |
| 9   | A     | 1134 | G    |
| 9   | A     | 1135 | C    |
| 9   | A     | 1136 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 9   | A     | 1138 | C    |
| 9   | A     | 1153 | C    |
| 9   | A     | 1154 | U    |
| 9   | A     | 1170 | A    |
| 9   | A     | 1195 | A    |
| 9   | A     | 1204 | A    |
| 9   | A     | 1207 | G    |
| 9   | A     | 1208 | A    |
| 9   | A     | 1209 | A    |
| 9   | A     | 1215 | C    |
| 9   | A     | 1216 | C    |
| 9   | A     | 1217 | A    |
| 9   | A     | 1220 | A    |
| 9   | A     | 1224 | G    |
| 9   | A     | 1225 | U    |
| 9   | A     | 1226 | G    |
| 9   | A     | 1227 | G    |
| 9   | A     | 1242 | U    |
| 9   | A     | 1243 | PSU  |
| 9   | A     | 1245 | G    |
| 9   | A     | 1250 | A    |
| 9   | A     | 1251 | A    |
| 9   | A     | 1253 | A    |
| 9   | A     | 1256 | G    |
| 9   | A     | 1257 | G    |
| 9   | A     | 1259 | A    |
| 9   | A     | 1274 | G    |
| 9   | A     | 1275 | G    |
| 9   | A     | 1284 | A    |
| 9   | A     | 1285 | G    |
| 9   | A     | 1286 | G    |
| 9   | A     | 1288 | U    |
| 9   | A     | 1292 | C    |
| 9   | A     | 1295 | A    |
| 9   | A     | 1301 | A    |
| 9   | A     | 1302 | G    |
| 9   | A     | 1303 | C    |
| 9   | A     | 1304 | U    |
| 9   | A     | 1305 | C    |
| 9   | A     | 1308 | U    |
| 9   | A     | 1309 | C    |
| 9   | A     | 1310 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 9   | A     | 1311 | C    |
| 9   | A     | 1312 | G    |
| 9   | A     | 1313 | A    |
| 9   | A     | 1314 | U    |
| 9   | A     | 1318 | G    |
| 9   | A     | 1322 | G    |
| 9   | A     | 1326 | U    |
| 9   | A     | 1342 | U    |
| 9   | A     | 1356 | G    |
| 9   | A     | 1357 | A    |
| 9   | A     | 1358 | U    |
| 9   | A     | 1371 | U    |
| 9   | A     | 1372 | U    |
| 9   | A     | 1378 | A    |
| 9   | A     | 1397 | U    |
| 9   | A     | 1402 | A    |
| 9   | A     | 1406 | G    |
| 9   | A     | 1417 | C    |
| 9   | A     | 1418 | C    |
| 9   | A     | 1419 | C    |
| 9   | A     | 1420 | G    |
| 9   | A     | 1421 | A    |
| 9   | A     | 1422 | G    |
| 9   | A     | 1423 | C    |
| 9   | A     | 1424 | G    |
| 9   | A     | 1433 | C    |
| 9   | A     | 1435 | C    |
| 9   | A     | 1436 | C    |
| 9   | A     | 1437 | C    |
| 9   | A     | 1438 | A    |
| 9   | A     | 1454 | A    |
| 9   | A     | 1455 | A    |
| 9   | A     | 1463 | U    |
| 9   | A     | 1489 | A    |
| 9   | A     | 1490 | G    |
| 9   | A     | 1496 | U    |
| 9   | A     | 1498 | A    |
| 9   | A     | 1519 | U    |
| 9   | A     | 1520 | G    |
| 9   | A     | 1521 | C    |
| 9   | A     | 1522 | A    |
| 9   | A     | 1533 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 9   | A     | 1534 | C    |
| 9   | A     | 1544 | C    |
| 9   | A     | 1556 | A    |
| 9   | A     | 1570 | G    |
| 9   | A     | 1580 | A    |
| 9   | A     | 1587 | G    |
| 9   | A     | 1588 | A    |
| 9   | A     | 1594 | A    |
| 9   | A     | 1598 | G    |
| 9   | A     | 1599 | U    |
| 9   | A     | 1600 | G    |
| 9   | A     | 1601 | A    |
| 9   | A     | 1602 | U    |
| 9   | A     | 1603 | G    |
| 9   | A     | 1604 | G    |
| 9   | A     | 1619 | A    |
| 9   | A     | 1621 | U    |
| 9   | A     | 1623 | A    |
| 9   | A     | 1624 | U    |
| 9   | A     | 1638 | G    |
| 9   | A     | 1639 | G    |
| 9   | A     | 1644 | C    |
| 9   | A     | 1648 | G    |
| 9   | A     | 1654 | G    |
| 9   | A     | 1663 | A    |
| 9   | A     | 1665 | G    |
| 9   | A     | 1671 | G    |
| 9   | A     | 1686 | G    |
| 9   | A     | 1687 | C    |
| 9   | A     | 1695 | A    |
| 9   | A     | 1699 | A    |
| 9   | A     | 1700 | C    |
| 9   | A     | 1701 | C    |
| 9   | A     | 1702 | G    |
| 9   | A     | 1711 | U    |
| 9   | A     | 1712 | A    |
| 9   | A     | 1715 | A    |
| 9   | A     | 1719 | A    |
| 9   | A     | 1721 | U    |
| 9   | A     | 1722 | G    |
| 9   | A     | 1733 | U    |
| 9   | A     | 1744 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 9   | A     | 1745 | A    |
| 9   | A     | 1749 | G    |
| 9   | A     | 1750 | C    |
| 9   | A     | 1752 | C    |
| 9   | A     | 1753 | C    |
| 9   | A     | 1754 | G    |
| 9   | A     | 1755 | C    |
| 9   | A     | 1756 | C    |
| 9   | A     | 1757 | G    |
| 9   | A     | 1758 | G    |
| 9   | A     | 1759 | G    |
| 9   | A     | 1760 | G    |
| 9   | A     | 1772 | C    |
| 9   | A     | 1773 | C    |
| 9   | A     | 1774 | C    |
| 9   | A     | 1775 | U    |
| 9   | A     | 1776 | G    |
| 9   | A     | 1777 | G    |
| 9   | A     | 1778 | C    |
| 9   | A     | 1779 | G    |
| 9   | A     | 1780 | G    |
| 9   | A     | 1781 | A    |
| 9   | A     | 1782 | G    |
| 9   | A     | 1783 | C    |
| 9   | A     | 1784 | G    |
| 9   | A     | 1800 | A    |
| 9   | A     | 1804 | U    |
| 9   | A     | 1805 | G    |
| 9   | A     | 1808 | U    |
| 9   | A     | 1809 | A    |
| 9   | A     | 1813 | A    |
| 9   | A     | 1819 | A    |
| 9   | A     | 1822 | A    |
| 9   | A     | 1823 | A    |
| 9   | A     | 1824 | A    |
| 9   | A     | 1825 | A    |
| 9   | A     | 1829 | G    |
| 9   | A     | 1834 | A    |
| 9   | A     | 1835 | A    |
| 9   | A     | 1837 | G    |
| 9   | A     | 1838 | U    |
| 9   | A     | 1839 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 9   | A     | 1841 | C    |
| 9   | A     | 1849 | G    |
| 9   | A     | 1851 | MA6  |
| 9   | A     | 1853 | C    |
| 9   | A     | 1860 | A    |
| 9   | A     | 1861 | G    |
| 9   | A     | 1862 | G    |
| 9   | A     | 1863 | A    |
| 9   | A     | 1864 | U    |
| 9   | A     | 1865 | C    |
| 9   | A     | 1867 | U    |
| 9   | A     | 1868 | U    |
| 9   | A     | 1869 | A    |
| 51  | w     | 2    | G    |
| 51  | w     | 3    | C    |
| 51  | w     | 6    | A    |
| 51  | w     | 7    | G    |
| 51  | w     | 8    | U    |
| 51  | w     | 9    | G    |
| 51  | w     | 10   | G    |
| 51  | w     | 14   | A    |
| 51  | w     | 15   | G    |
| 51  | w     | 16   | C    |
| 51  | w     | 17   | G    |
| 51  | w     | 18   | G    |
| 51  | w     | 19   | A    |
| 51  | w     | 20   | A    |
| 51  | w     | 28   | G    |
| 51  | w     | 29   | G    |
| 51  | w     | 34   | A    |
| 51  | w     | 36   | A    |
| 51  | w     | 38   | C    |
| 51  | w     | 39   | C    |
| 51  | w     | 40   | C    |
| 51  | w     | 42   | G    |
| 51  | w     | 43   | A    |
| 51  | w     | 44   | G    |
| 51  | w     | 45   | G    |
| 51  | w     | 46   | U    |
| 51  | w     | 51   | G    |
| 51  | w     | 52   | G    |
| 51  | w     | 54   | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 51  | w     | 55  | C    |
| 51  | w     | 56  | G    |
| 51  | w     | 57  | A    |
| 51  | w     | 58  | A    |
| 51  | w     | 60  | C    |
| 51  | w     | 63  | U    |
| 51  | w     | 64  | C    |
| 51  | w     | 70  | C    |
| 51  | w     | 71  | U    |
| 51  | w     | 73  | C    |
| 51  | w     | 74  | C    |
| 51  | w     | 75  | A    |

All (52) RNA pucker outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 9   | A     | 1    | U    |
| 9   | A     | 9    | U    |
| 9   | A     | 196  | C    |
| 9   | A     | 197  | U    |
| 9   | A     | 201  | C    |
| 9   | A     | 203  | G    |
| 9   | A     | 291  | G    |
| 9   | A     | 293  | C    |
| 9   | A     | 366  | U    |
| 9   | A     | 368  | U    |
| 9   | A     | 370  | G    |
| 9   | A     | 371  | A    |
| 9   | A     | 392  | A    |
| 9   | A     | 393  | U    |
| 9   | A     | 396  | U    |
| 9   | A     | 686  | U    |
| 9   | A     | 687  | C    |
| 9   | A     | 688  | U    |
| 9   | A     | 797  | C    |
| 9   | A     | 798  | G    |
| 9   | A     | 838  | G    |
| 9   | A     | 839  | C    |
| 9   | A     | 989  | C    |
| 9   | A     | 1250 | A    |
| 9   | A     | 1286 | G    |
| 9   | A     | 1301 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 9   | A     | 1304 | U    |
| 9   | A     | 1312 | G    |
| 9   | A     | 1313 | A    |
| 9   | A     | 1434 | C    |
| 9   | A     | 1519 | U    |
| 9   | A     | 1520 | G    |
| 9   | A     | 1521 | C    |
| 9   | A     | 1598 | G    |
| 9   | A     | 1599 | U    |
| 9   | A     | 1600 | G    |
| 9   | A     | 1601 | A    |
| 9   | A     | 1603 | G    |
| 9   | A     | 1699 | A    |
| 9   | A     | 1700 | C    |
| 9   | A     | 1701 | C    |
| 9   | A     | 1744 | G    |
| 9   | A     | 1753 | C    |
| 9   | A     | 1759 | G    |
| 9   | A     | 1775 | U    |
| 9   | A     | 1781 | A    |
| 9   | A     | 1824 | A    |
| 9   | A     | 1834 | A    |
| 9   | A     | 1862 | G    |
| 9   | A     | 1863 | A    |
| 9   | A     | 1867 | U    |
| 9   | A     | 1868 | U    |

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

26 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 |
| 9   | A2M  | A     | 159  | 9    | 22,25,26     | 0.98 | 2 (9%)   | 30,36,39    | 0.97 | 3 (10%)  |
| 9   | PSU  | A     | 1243 | 9    | 18,21,22     | 1.29 | 2 (11%)  | 21,30,33    | 1.11 | 2 (9%)   |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 9   | A2M  | A     | 1678 | 9    | 22,25,26     | 0.77 | 0        | 30,36,39    | 0.98 | 2 (6%)   |
| 9   | A2M  | A     | 27   | 9    | 22,25,26     | 0.94 | 1 (4%)   | 30,36,39    | 0.90 | 1 (3%)   |
| 9   | PSU  | A     | 119  | 9    | 18,21,22     | 1.13 | 2 (11%)  | 21,30,33    | 1.22 | 3 (14%)  |
| 9   | 5MC  | A     | 1374 | 9    | 19,22,23     | 0.68 | 0        | 26,32,35    | 0.62 | 0        |
| 9   | OMC  | A     | 174  | 9    | 19,22,23     | 0.59 | 0        | 25,31,34    | 0.45 | 0        |
| 9   | A2M  | A     | 668  | 9    | 22,25,26     | 1.02 | 2 (9%)   | 30,36,39    | 0.97 | 1 (3%)   |
| 9   | OMC  | A     | 1703 | 9    | 19,22,23     | 0.70 | 0        | 25,31,34    | 0.52 | 0        |
| 9   | UR3  | A     | 1830 | 9    | 19,22,23     | 0.98 | 1 (5%)   | 26,32,35    | 2.11 | 6 (23%)  |
| 9   | MA6  | A     | 1850 | 9    | 23,26,27     | 0.98 | 1 (4%)   | 33,38,41    | 1.41 | 3 (9%)   |
| 9   | A2M  | A     | 484  | 9    | 22,25,26     | 0.86 | 1 (4%)   | 30,36,39    | 0.96 | 2 (6%)   |
| 9   | MA6  | A     | 1851 | 9    | 23,26,27     | 0.92 | 2 (8%)   | 33,38,41    | 1.22 | 2 (6%)   |
| 9   | OMU  | A     | 116  | 9    | 19,22,23     | 0.73 | 0        | 25,31,34    | 0.82 | 0        |
| 9   | OMC  | A     | 517  | 9    | 19,22,23     | 0.59 | 0        | 25,31,34    | 0.46 | 0        |
| 9   | A2M  | A     | 1031 | 9    | 22,25,26     | 0.98 | 2 (9%)   | 30,36,39    | 0.89 | 1 (3%)   |
| 9   | PSU  | A     | 823  | 9    | 18,21,22     | 1.17 | 2 (11%)  | 21,30,33    | 1.21 | 2 (9%)   |
| 9   | OMU  | A     | 121  | 9    | 19,22,23     | 0.88 | 0        | 25,31,34    | 0.89 | 1 (4%)   |
| 9   | A2M  | A     | 166  | 9    | 22,25,26     | 0.83 | 1 (4%)   | 30,36,39    | 1.12 | 2 (6%)   |
| 9   | OMG  | A     | 644  | 9    | 23,26,27     | 0.82 | 0        | 32,38,41    | 0.73 | 0        |
| 9   | PSU  | A     | 612  | 9    | 18,21,22     | 1.08 | 1 (5%)   | 21,30,33    | 1.00 | 1 (4%)   |
| 9   | PSU  | A     | 1081 | 9    | 18,21,22     | 1.13 | 1 (5%)   | 21,30,33    | 1.20 | 2 (9%)   |
| 9   | OMG  | A     | 683  | 9    | 23,26,27     | 0.90 | 1 (4%)   | 32,38,41    | 0.89 | 1 (3%)   |
| 9   | 5MU  | A     | 814  | 9    | 19,22,23     | 0.92 | 1 (5%)   | 27,32,35    | 0.94 | 1 (3%)   |
| 9   | OMG  | A     | 509  | 9    | 23,26,27     | 1.29 | 3 (13%)  | 32,38,41    | 2.15 | 7 (21%)  |
| 9   | PSU  | A     | 822  | 9    | 18,21,22     | 1.13 | 1 (5%)   | 21,30,33    | 1.18 | 2 (9%)   |

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   |
|-----|------|-------|------|------|---------|-----------|---------|
| 9   | A2M  | A     | 159  | 9    | -       | 2/9/27/28 | 0/3/3/3 |
| 9   | PSU  | A     | 1243 | 9    | -       | 0/7/25/26 | 0/2/2/2 |
| 9   | A2M  | A     | 1678 | 9    | -       | 0/9/27/28 | 0/3/3/3 |
| 9   | A2M  | A     | 27   | 9    | -       | 0/9/27/28 | 0/3/3/3 |
| 9   | PSU  | A     | 119  | 9    | -       | 0/7/25/26 | 0/2/2/2 |
| 9   | 5MC  | A     | 1374 | 9    | -       | 0/7/25/26 | 0/2/2/2 |
| 9   | OMC  | A     | 174  | 9    | -       | 0/9/27/28 | 0/2/2/2 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 9   | A2M  | A     | 668  | 9    | -       | 2/9/27/28  | 0/3/3/3 |
| 9   | OMC  | A     | 1703 | 9    | -       | 0/9/27/28  | 0/2/2/2 |
| 9   | UR3  | A     | 1830 | 9    | -       | 2/7/25/26  | 0/2/2/2 |
| 9   | MA6  | A     | 1850 | 9    | -       | 3/11/29/30 | 0/3/3/3 |
| 9   | A2M  | A     | 484  | 9    | -       | 0/9/27/28  | 0/3/3/3 |
| 9   | MA6  | A     | 1851 | 9    | -       | 5/11/29/30 | 0/3/3/3 |
| 9   | OMU  | A     | 116  | 9    | -       | 1/9/27/28  | 0/2/2/2 |
| 9   | OMC  | A     | 517  | 9    | -       | 1/9/27/28  | 0/2/2/2 |
| 9   | A2M  | A     | 1031 | 9    | -       | 0/9/27/28  | 0/3/3/3 |
| 9   | PSU  | A     | 823  | 9    | -       | 0/7/25/26  | 0/2/2/2 |
| 9   | OMU  | A     | 121  | 9    | -       | 0/9/27/28  | 0/2/2/2 |
| 9   | A2M  | A     | 166  | 9    | -       | 0/9/27/28  | 0/3/3/3 |
| 9   | OMG  | A     | 644  | 9    | -       | 2/9/27/28  | 0/3/3/3 |
| 9   | PSU  | A     | 612  | 9    | -       | 0/7/25/26  | 0/2/2/2 |
| 9   | PSU  | A     | 1081 | 9    | -       | 1/7/25/26  | 0/2/2/2 |
| 9   | OMG  | A     | 683  | 9    | -       | 0/9/27/28  | 0/3/3/3 |
| 9   | 5MU  | A     | 814  | 9    | -       | 0/7/25/26  | 0/2/2/2 |
| 9   | OMG  | A     | 509  | 9    | -       | 1/9/27/28  | 0/3/3/3 |
| 9   | PSU  | A     | 822  | 9    | -       | 0/7/25/26  | 0/2/2/2 |

All (27) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 9   | A     | 1243 | PSU  | C6-C5   | 3.56  | 1.39        | 1.35     |
| 9   | A     | 822  | PSU  | C6-C5   | 3.52  | 1.39        | 1.35     |
| 9   | A     | 119  | PSU  | C6-C5   | 3.45  | 1.39        | 1.35     |
| 9   | A     | 823  | PSU  | C6-C5   | 3.04  | 1.38        | 1.35     |
| 9   | A     | 509  | OMG  | C5-C4   | 2.98  | 1.46        | 1.38     |
| 9   | A     | 509  | OMG  | C6-N1   | -2.96 | 1.33        | 1.38     |
| 9   | A     | 668  | A2M  | C5-N7   | -2.91 | 1.33        | 1.39     |
| 9   | A     | 1081 | PSU  | C6-C5   | 2.74  | 1.38        | 1.35     |
| 9   | A     | 1031 | A2M  | C5-N7   | -2.67 | 1.34        | 1.39     |
| 9   | A     | 1850 | MA6  | C5-N7   | -2.58 | 1.34        | 1.39     |
| 9   | A     | 509  | OMG  | C5-N7   | -2.52 | 1.34        | 1.39     |
| 9   | A     | 612  | PSU  | C6-C5   | 2.50  | 1.38        | 1.35     |
| 9   | A     | 159  | A2M  | C5-N7   | -2.49 | 1.34        | 1.39     |
| 9   | A     | 27   | A2M  | C5-N7   | -2.41 | 1.34        | 1.39     |
| 9   | A     | 1851 | MA6  | C5-N7   | -2.39 | 1.34        | 1.39     |
| 9   | A     | 1243 | PSU  | C2'-C1' | -2.28 | 1.50        | 1.53     |
| 9   | A     | 1851 | MA6  | C5-C4   | 2.22  | 1.43        | 1.39     |
| 9   | A     | 668  | A2M  | C5-C4   | 2.21  | 1.43        | 1.39     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 9   | A     | 683  | OMG  | C6-N1 | -2.17 | 1.34        | 1.38     |
| 9   | A     | 119  | PSU  | C4-N3 | -2.15 | 1.34        | 1.38     |
| 9   | A     | 166  | A2M  | C5-C4 | 2.15  | 1.42        | 1.39     |
| 9   | A     | 814  | 5MU  | C4-N3 | -2.15 | 1.34        | 1.38     |
| 9   | A     | 484  | A2M  | C5-N7 | -2.14 | 1.35        | 1.39     |
| 9   | A     | 823  | PSU  | C4-N3 | -2.13 | 1.34        | 1.38     |
| 9   | A     | 1830 | UR3  | C5-C4 | -2.11 | 1.38        | 1.43     |
| 9   | A     | 159  | A2M  | C4-N9 | -2.05 | 1.33        | 1.37     |
| 9   | A     | 1031 | A2M  | C8-N9 | -2.04 | 1.34        | 1.37     |

All (45) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 9   | A     | 1830 | UR3  | C4-N3-C2    | -6.53 | 119.32      | 124.58   |
| 9   | A     | 509  | OMG  | C5-C4-N3    | -6.32 | 118.33      | 128.39   |
| 9   | A     | 509  | OMG  | C2'-C1'-N9  | -4.95 | 104.84      | 114.24   |
| 9   | A     | 509  | OMG  | C2-N3-C4    | 4.69  | 120.38      | 112.30   |
| 9   | A     | 509  | OMG  | N9-C4-N3    | 4.64  | 135.24      | 125.95   |
| 9   | A     | 1850 | MA6  | N1-C6-N6    | 3.80  | 121.49      | 116.86   |
| 9   | A     | 1830 | UR3  | C5-C4-N3    | 3.78  | 120.03      | 115.04   |
| 9   | A     | 1850 | MA6  | C5-C6-N6    | -3.77 | 119.37      | 125.33   |
| 9   | A     | 1830 | UR3  | C1'-N1-C2   | 3.59  | 122.91      | 117.04   |
| 9   | A     | 1850 | MA6  | C2-N1-C6    | 3.42  | 120.18      | 111.83   |
| 9   | A     | 1851 | MA6  | C2-N1-C6    | 3.31  | 119.93      | 111.83   |
| 9   | A     | 1830 | UR3  | O4'-C1'-N1  | 3.20  | 115.60      | 108.36   |
| 9   | A     | 1081 | PSU  | C6-C5-C4    | -3.14 | 116.06      | 118.17   |
| 9   | A     | 823  | PSU  | N1-C2-N3    | 3.10  | 118.44      | 115.17   |
| 9   | A     | 1830 | UR3  | O3'-C3'-C2' | -3.06 | 102.02      | 111.82   |
| 9   | A     | 119  | PSU  | C6-C5-C4    | -2.88 | 116.23      | 118.17   |
| 9   | A     | 119  | PSU  | N1-C2-N3    | 2.71  | 118.03      | 115.17   |
| 9   | A     | 1243 | PSU  | N1-C2-N3    | 2.70  | 118.02      | 115.17   |
| 9   | A     | 166  | A2M  | C4-N9-C8    | 2.69  | 108.56      | 105.74   |
| 9   | A     | 509  | OMG  | C6-C5-N7    | 2.66  | 135.13      | 130.29   |
| 9   | A     | 1678 | A2M  | C4-N9-C8    | 2.56  | 108.43      | 105.74   |
| 9   | A     | 159  | A2M  | N3-C4-N9    | 2.51  | 131.44      | 127.17   |
| 9   | A     | 166  | A2M  | N3-C4-N9    | 2.48  | 131.39      | 127.17   |
| 9   | A     | 484  | A2M  | N3-C4-N9    | 2.48  | 131.38      | 127.17   |
| 9   | A     | 159  | A2M  | C5-C4-N3    | -2.36 | 123.47      | 126.72   |
| 9   | A     | 814  | 5MU  | O4-C4-C5    | -2.32 | 122.26      | 124.92   |
| 9   | A     | 1081 | PSU  | C3'-C2'-C1' | 2.30  | 104.41      | 101.69   |
| 9   | A     | 509  | OMG  | C4-C5-N7    | -2.30 | 107.02      | 110.67   |
| 9   | A     | 823  | PSU  | C6-C5-C4    | -2.27 | 116.64      | 118.17   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 9   | A     | 822  | PSU  | N1-C2-N3    | 2.27  | 117.56      | 115.17   |
| 9   | A     | 509  | OMG  | O6-C6-C5    | -2.25 | 120.59      | 126.53   |
| 9   | A     | 484  | A2M  | C4-N9-C8    | 2.24  | 108.08      | 105.74   |
| 9   | A     | 668  | A2M  | C4-N9-C8    | 2.22  | 108.07      | 105.74   |
| 9   | A     | 1243 | PSU  | O2-C2-N1    | -2.15 | 120.57      | 122.79   |
| 9   | A     | 1678 | A2M  | N3-C4-N9    | 2.15  | 130.82      | 127.17   |
| 9   | A     | 822  | PSU  | O2'-C2'-C1' | -2.13 | 106.17      | 111.21   |
| 9   | A     | 119  | PSU  | O2-C2-N1    | -2.12 | 120.60      | 122.79   |
| 9   | A     | 612  | PSU  | N1-C2-N3    | 2.12  | 117.40      | 115.17   |
| 9   | A     | 159  | A2M  | C4-N9-C8    | 2.11  | 107.96      | 105.74   |
| 9   | A     | 1851 | MA6  | C5-C6-N6    | -2.09 | 122.03      | 125.33   |
| 9   | A     | 683  | OMG  | N9-C4-N3    | 2.05  | 130.05      | 125.95   |
| 9   | A     | 121  | OMU  | N3-C2-N1    | 2.04  | 117.55      | 114.89   |
| 9   | A     | 1031 | A2M  | N3-C4-N9    | 2.04  | 130.64      | 127.17   |
| 9   | A     | 27   | A2M  | C4-N9-C8    | 2.01  | 107.85      | 105.74   |
| 9   | A     | 1830 | UR3  | C3U-N3-C2   | 2.01  | 120.83      | 117.33   |

There are no chirality outliers.

All (20) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 9   | A     | 509  | OMG  | C1'-C2'-O2'-CM2 |
| 9   | A     | 1830 | UR3  | O4'-C1'-N1-C6   |
| 9   | A     | 1830 | UR3  | O4'-C1'-N1-C2   |
| 9   | A     | 1850 | MA6  | C5-C6-N6-C10    |
| 9   | A     | 1851 | MA6  | O4'-C4'-C5'-O5' |
| 9   | A     | 1851 | MA6  | C5-C6-N6-C10    |
| 9   | A     | 1850 | MA6  | N1-C6-N6-C10    |
| 9   | A     | 1851 | MA6  | N1-C6-N6-C10    |
| 9   | A     | 1851 | MA6  | C3'-C4'-C5'-O5' |
| 9   | A     | 668  | A2M  | C3'-C4'-C5'-O5' |
| 9   | A     | 1851 | MA6  | C5-C6-N6-C9     |
| 9   | A     | 159  | A2M  | C3'-C4'-C5'-O5' |
| 9   | A     | 668  | A2M  | O4'-C4'-C5'-O5' |
| 9   | A     | 159  | A2M  | O4'-C4'-C5'-O5' |
| 9   | A     | 116  | OMU  | C1'-C2'-O2'-CM2 |
| 9   | A     | 1850 | MA6  | C5-C6-N6-C9     |
| 9   | A     | 1081 | PSU  | C4'-C5'-O5'-P   |
| 9   | A     | 517  | OMC  | C1'-C2'-O2'-CM2 |
| 9   | A     | 644  | OMG  | C4'-C5'-O5'-P   |
| 9   | A     | 644  | OMG  | C3'-C4'-C5'-O5' |

There are no ring outliers.

10 monomers are involved in 16 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 9   | A     | 159  | A2M  | 1       | 0            |
| 9   | A     | 1678 | A2M  | 2       | 0            |
| 9   | A     | 174  | OMC  | 1       | 0            |
| 9   | A     | 1703 | OMC  | 1       | 0            |
| 9   | A     | 116  | OMU  | 3       | 0            |
| 9   | A     | 517  | OMC  | 1       | 0            |
| 9   | A     | 1031 | A2M  | 3       | 0            |
| 9   | A     | 121  | OMU  | 1       | 0            |
| 9   | A     | 683  | OMG  | 1       | 0            |
| 9   | A     | 509  | OMG  | 2       | 0            |

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

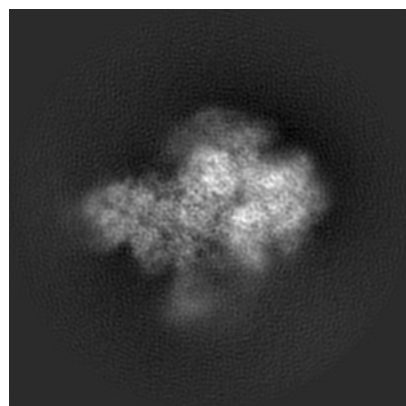
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14113. These allow visual inspection of the internal detail of the map and identification of artifacts.

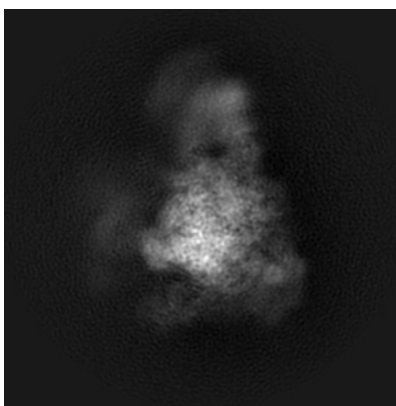
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

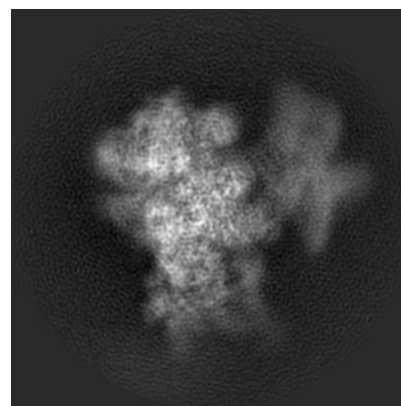
#### 6.1.1 Primary map



X

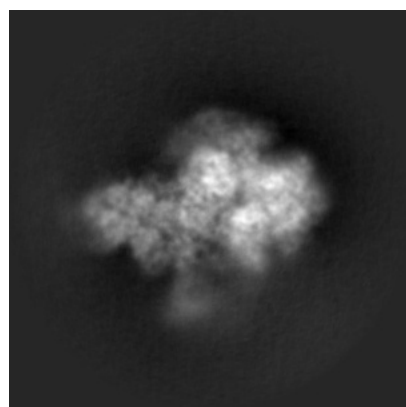


Y

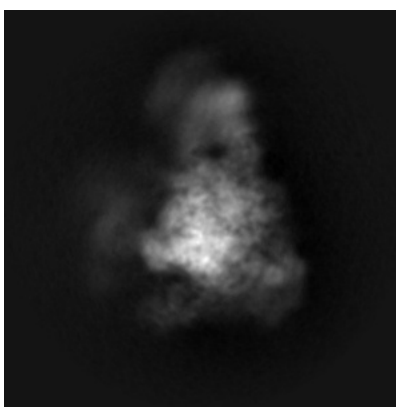


Z

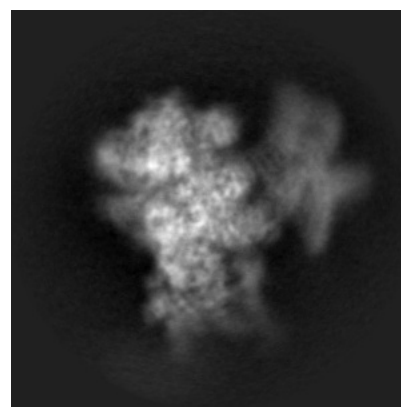
#### 6.1.2 Raw map



X



Y

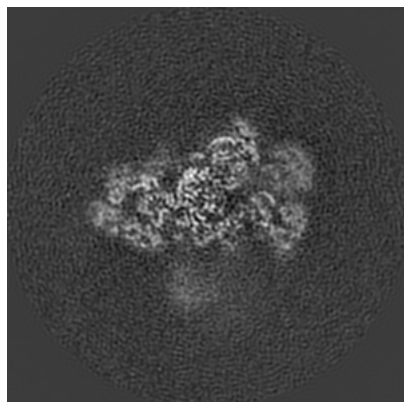


Z

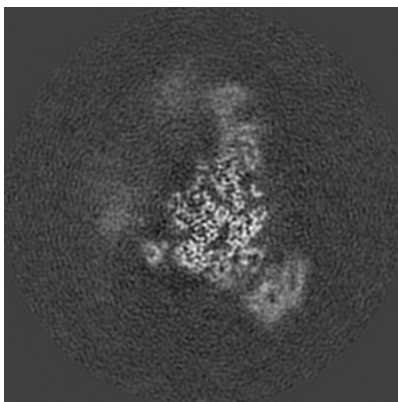
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

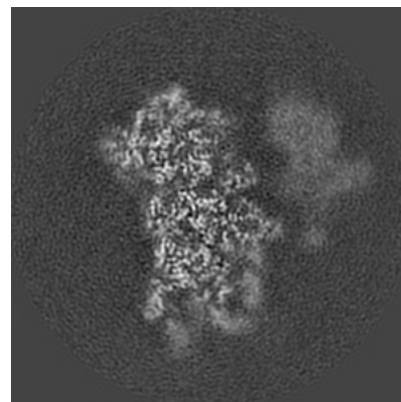
### 6.2.1 Primary map



X Index: 180

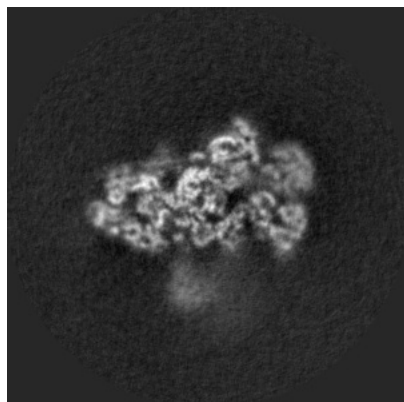


Y Index: 180

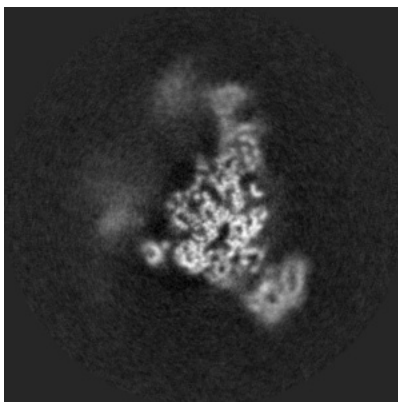


Z Index: 180

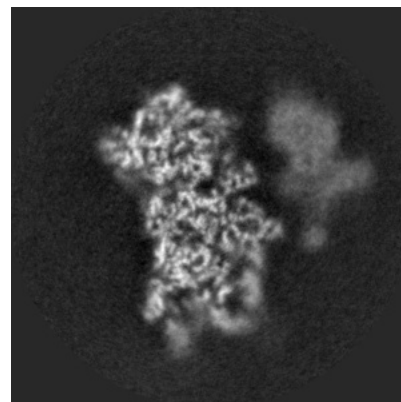
### 6.2.2 Raw map



X Index: 180



Y Index: 180

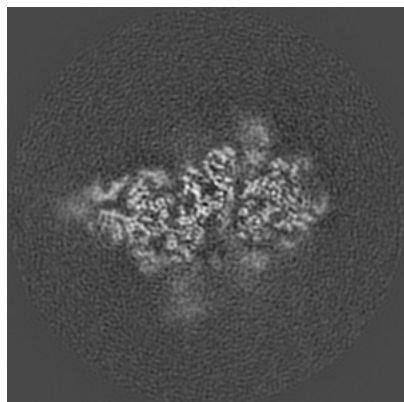


Z Index: 180

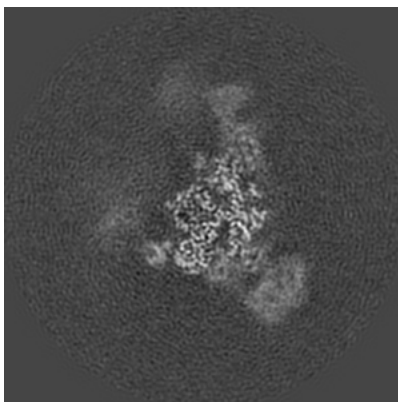
The images above show central slices of the map in three orthogonal directions.

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

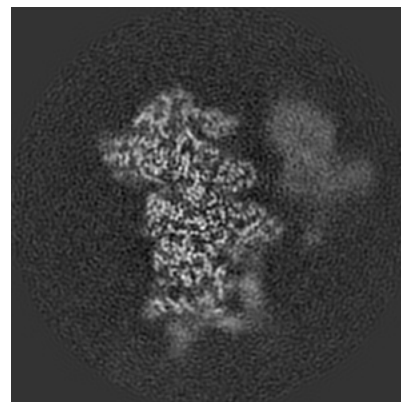
### 6.3.1 Primary map



X Index: 152

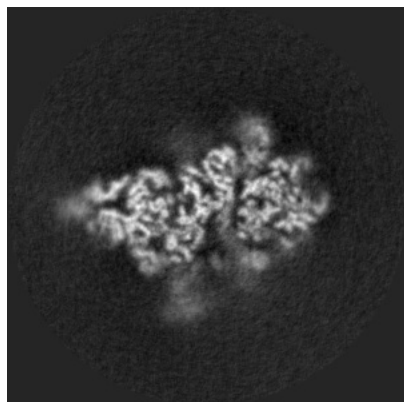


Y Index: 178

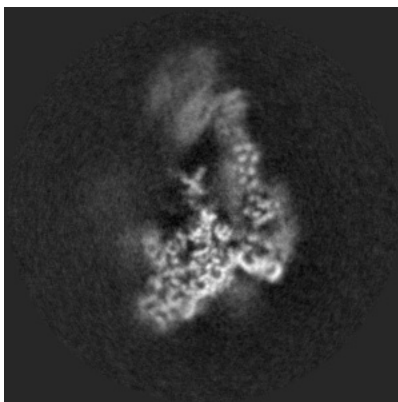


Z Index: 176

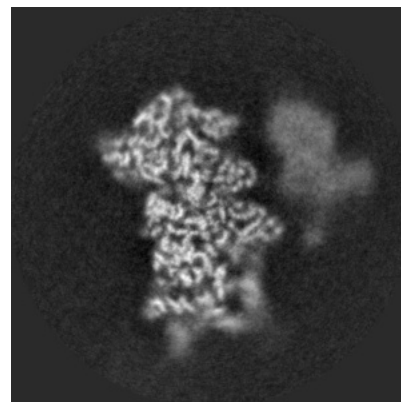
### 6.3.2 Raw map



X Index: 152



Y Index: 219

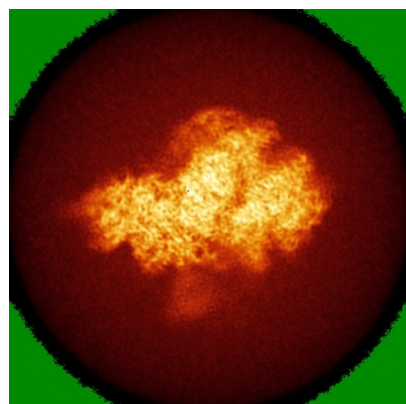


Z Index: 176

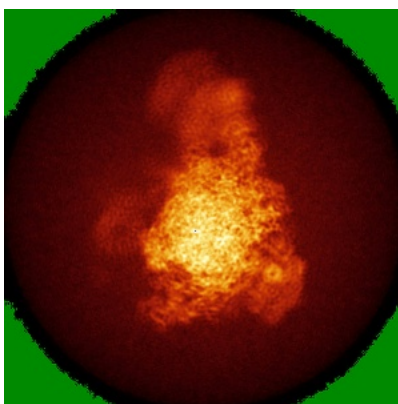
The images above show the largest variance slices of the map in three orthogonal directions.

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

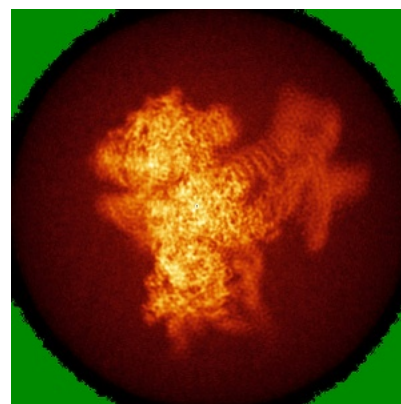
### 6.4.1 Primary map



X

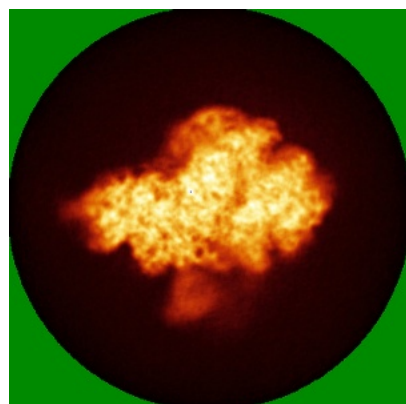


Y

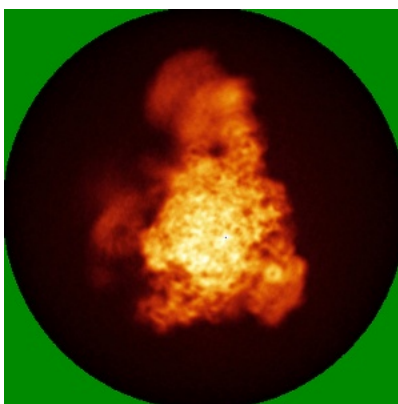


Z

### 6.4.2 Raw map



X



Y

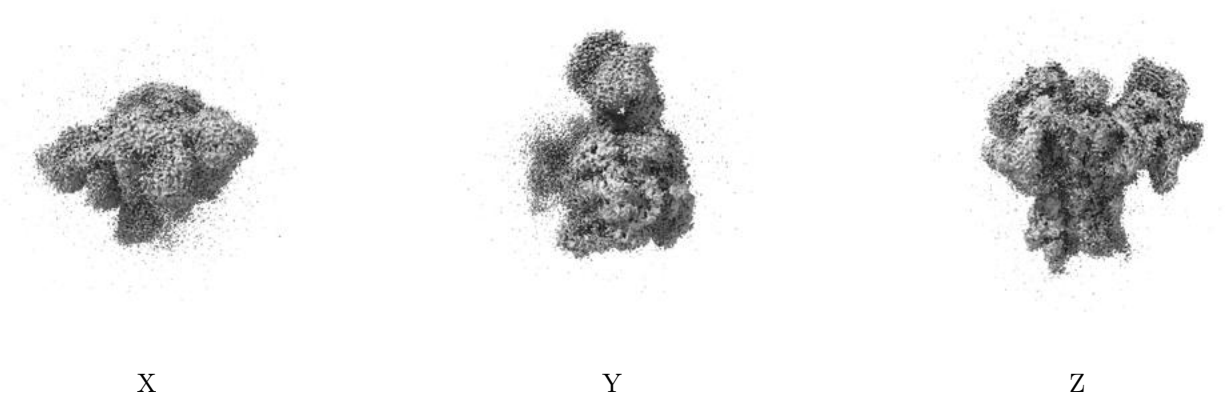


Z

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

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

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 2.3. 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 shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

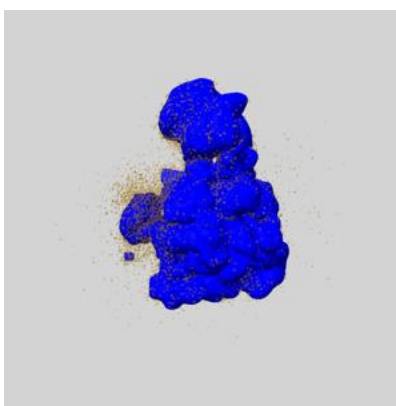
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

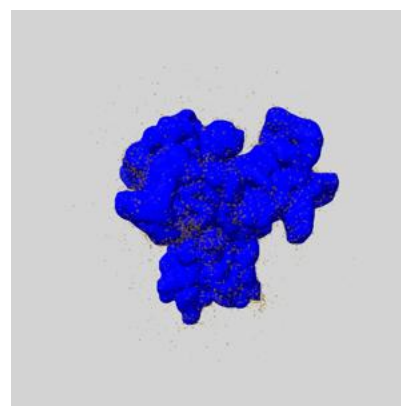
### 6.6.1 emd\_14113\_msk\_1.map [i](#)



X



Y

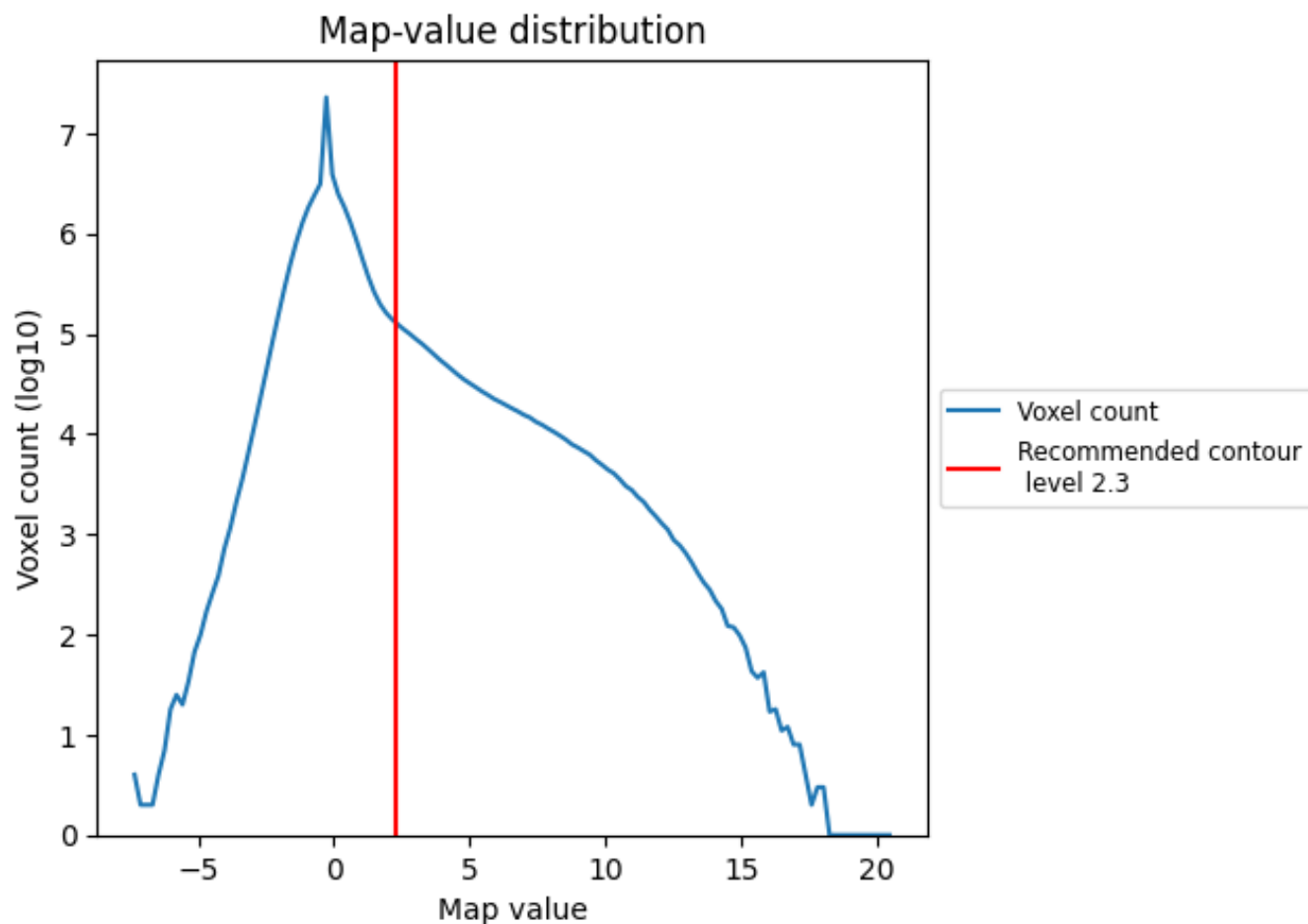


Z

## 7 Map analysis [i](#)

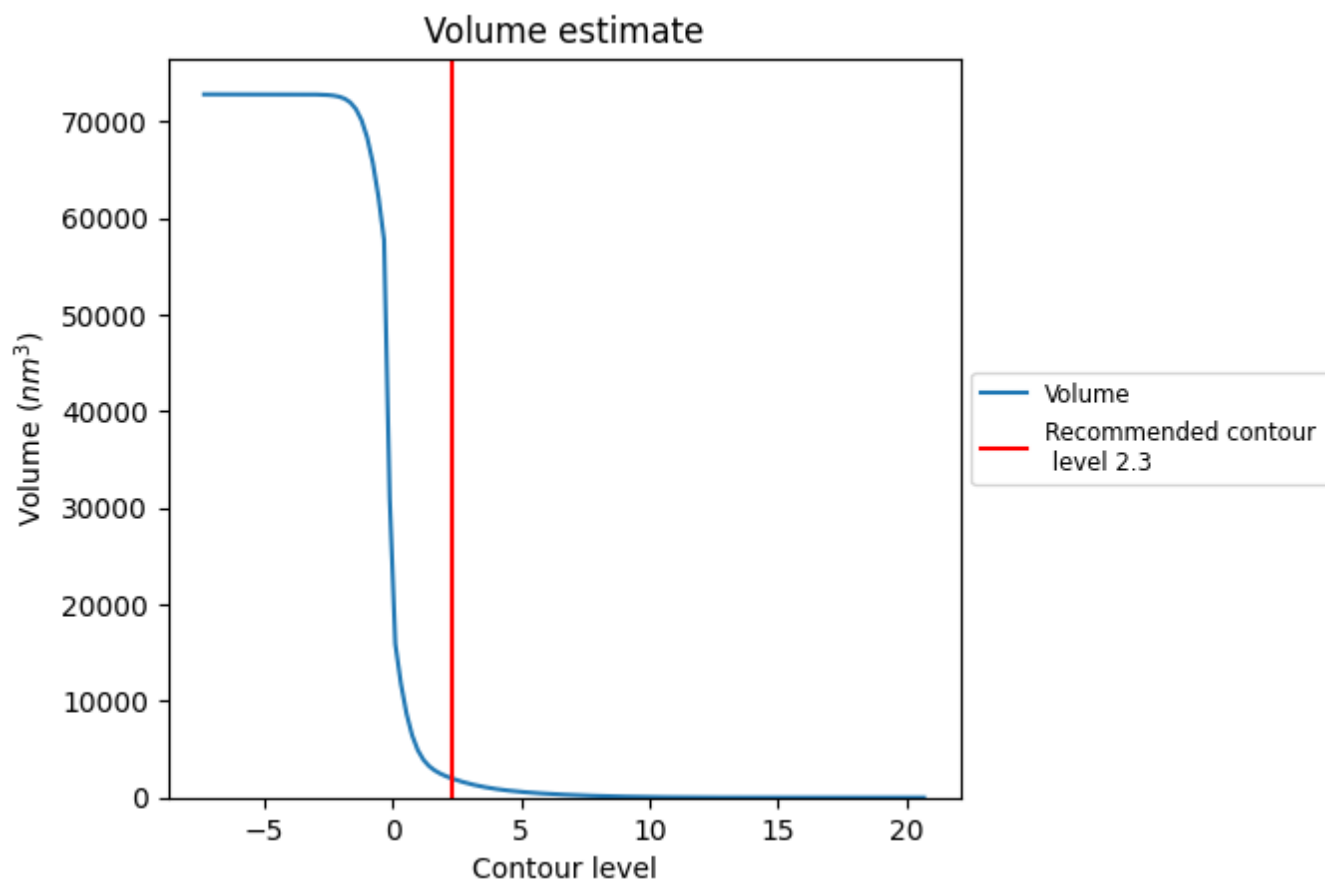
This section contains the results of statistical analysis of the map.

### 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.

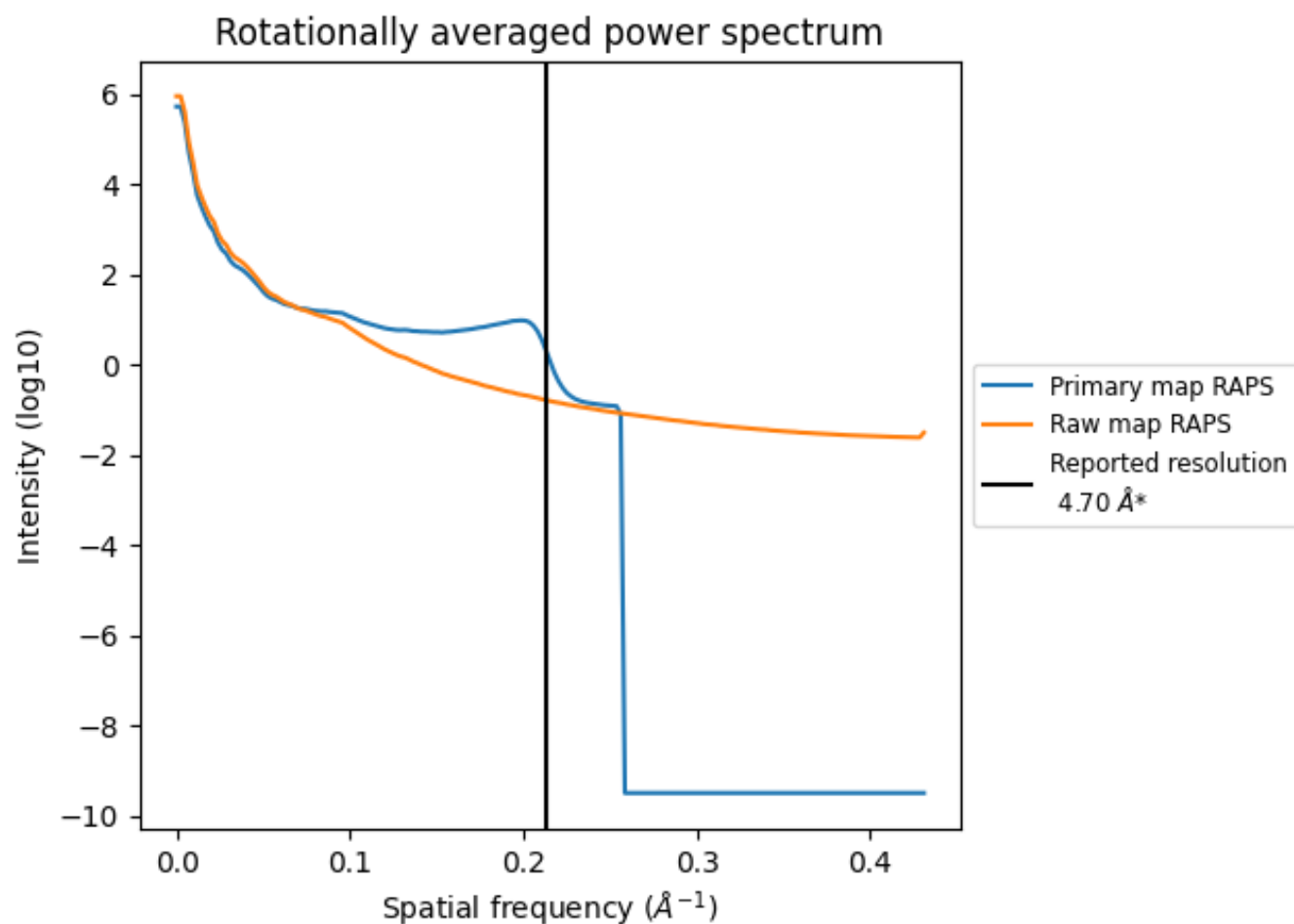
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1983 nm<sup>3</sup>; this corresponds to an approximate mass of 1791 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 ⓘ

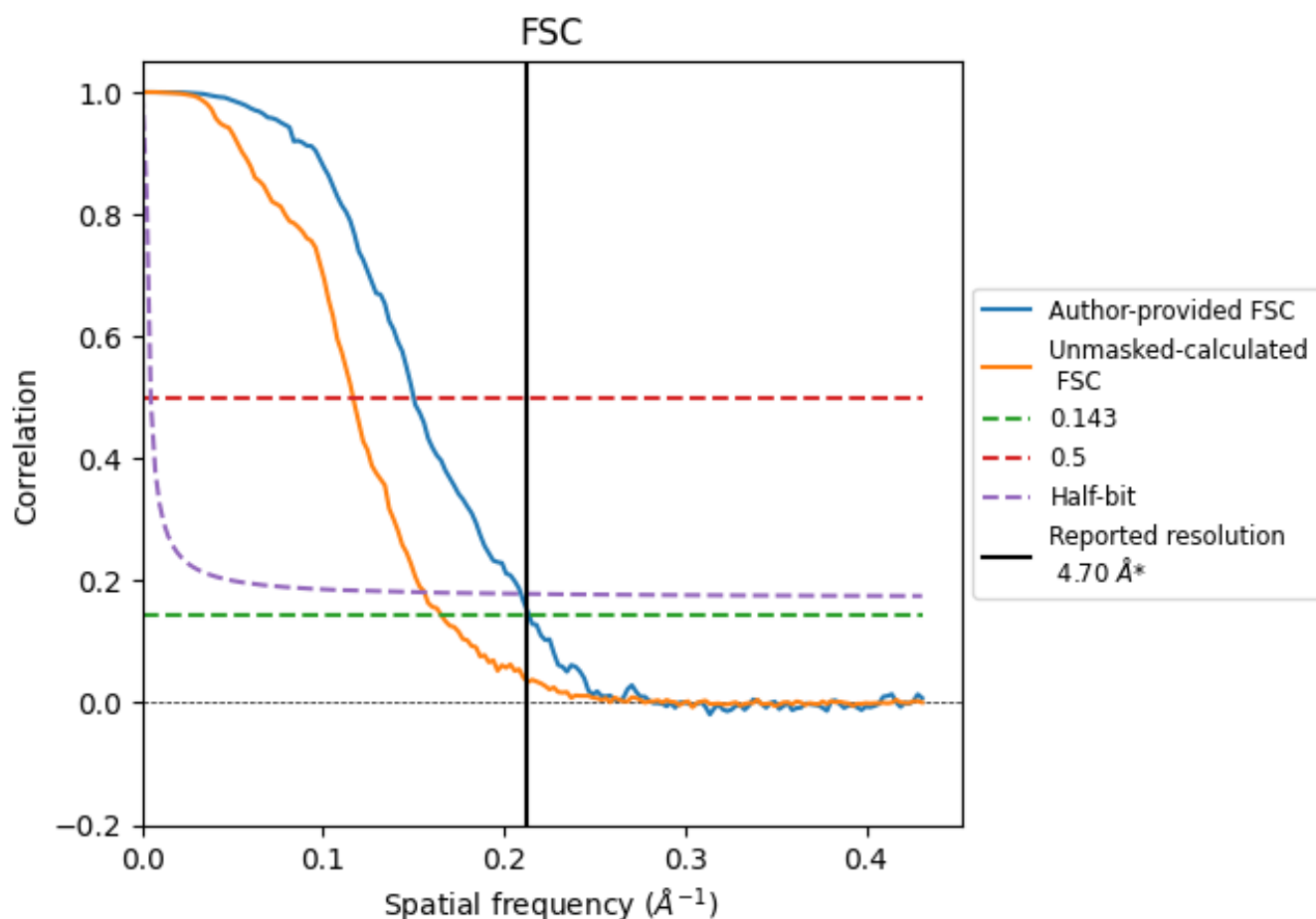


\*Reported resolution corresponds to spatial frequency of 0.213 Å<sup>-1</sup>

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.213  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

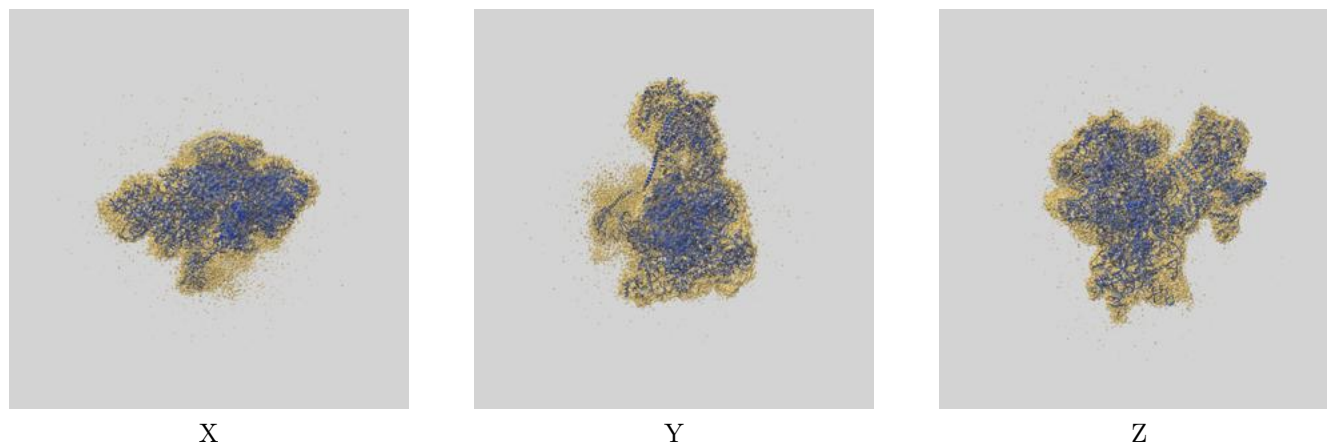
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 4.70                               | -    | -        |
| Author-provided FSC curve | 4.68                               | 6.67 | 4.78     |
| Unmasked-calculated*      | 6.05                               | 8.58 | 6.41     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.05 differs from the reported value 4.7 by more than 10 %

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

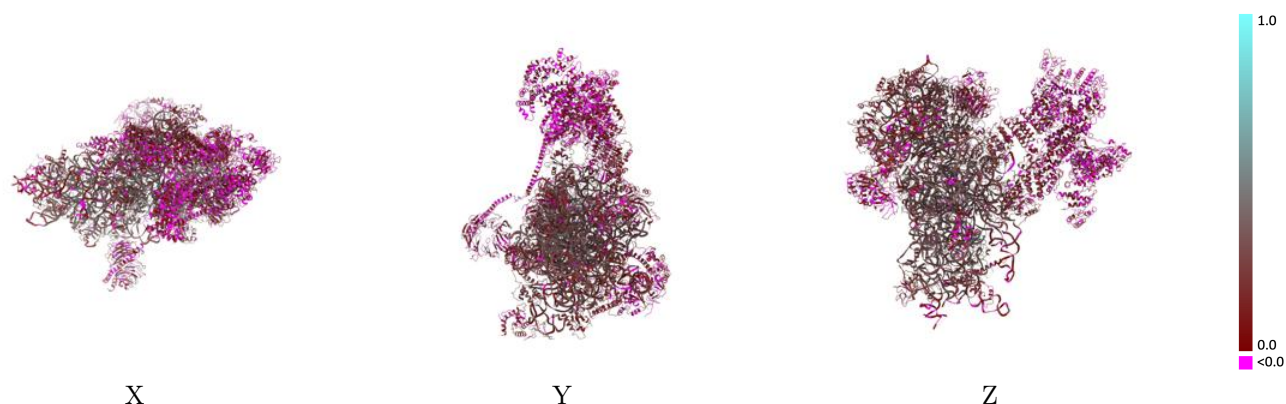
This section contains information regarding the fit between EMDB map EMD-14113 and PDB model 7QP6. Per-residue inclusion information can be found in section [3](#) on page [13](#).

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



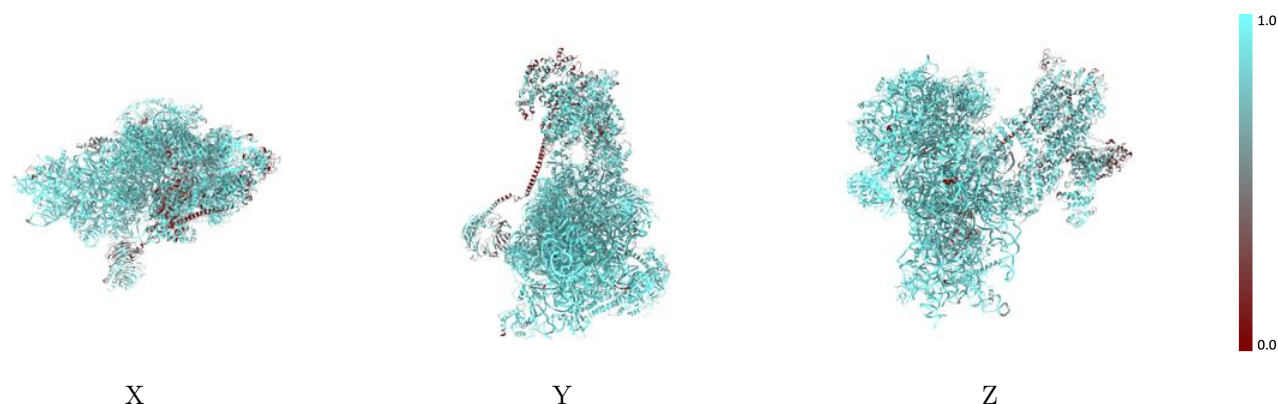
The images above show the 3D surface view of the map at the recommended contour level 2.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



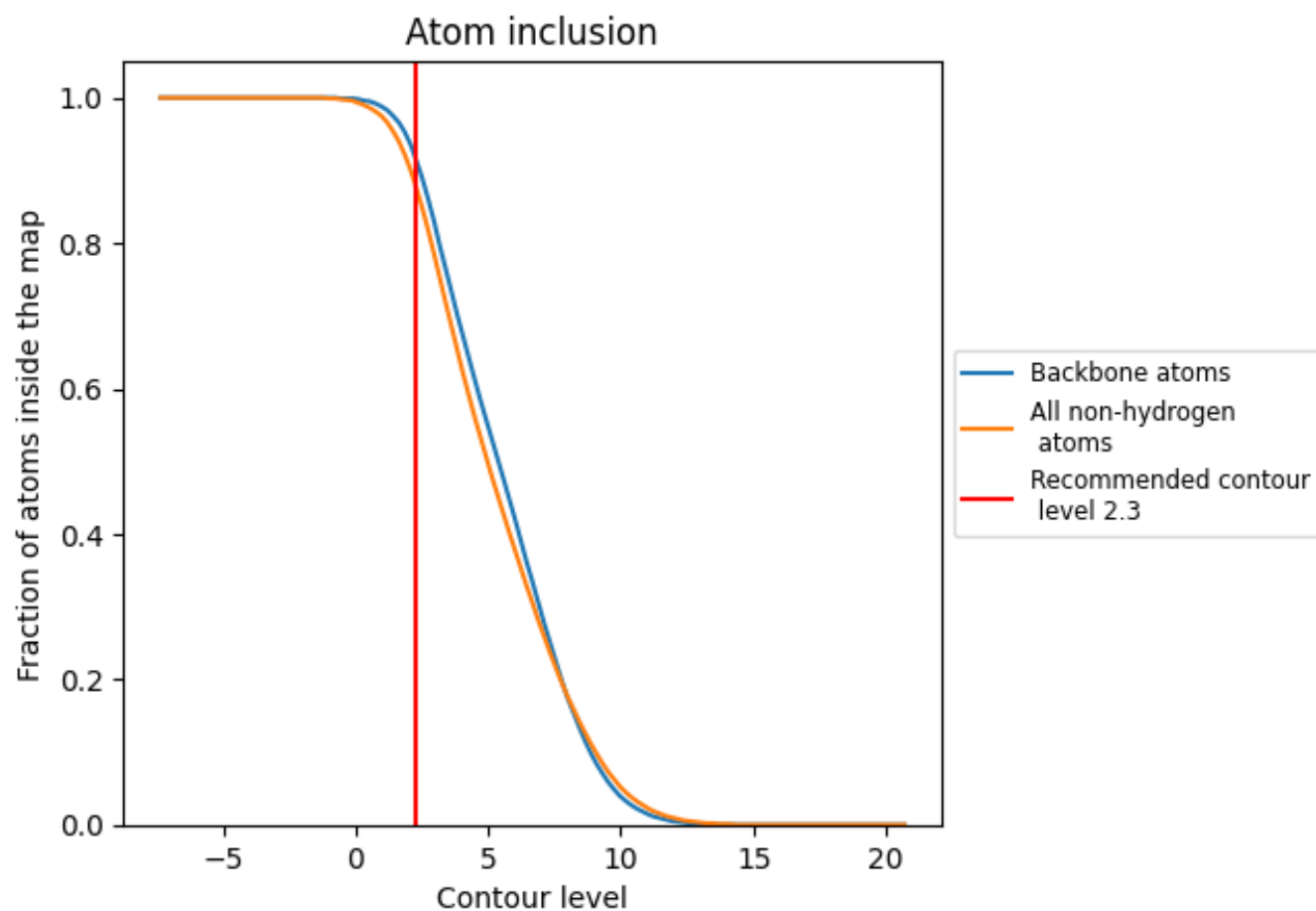
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (2.3).

## 9.4 Atom inclusion ⓘ



At the recommended contour level, 91% 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 (2.3) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.8750   |  0.2330   |
| 1     |  0.6150   |  0.1310   |
| 3     |  0.5170   |  0.0340   |
| 4     |  0.7820   |  0.0690   |
| 5     |  0.6800   |  0.0350   |
| 6     |  0.6940   |  0.0470   |
| 7     |  0.7750   |  0.0750   |
| 8     |  0.6890   |  0.0500   |
| 9     |  0.9520   |  0.3600   |
| A     |  0.9790   |  0.3000   |
| B     |  0.9270   |  0.3770   |
| C     |  0.9190   |  0.3440   |
| D     |  0.8790   |  0.2860   |
| E     |  0.9050   |  0.3440   |
| F     |  0.9430  |  0.3260  |
| G     |  0.8620 |  0.2610 |
| H     |  0.8560 |  0.2960 |
| I     |  0.8970 |  0.3010 |
| J     |  0.8570 |  0.3270 |
| K     |  0.8760 |  0.3220 |
| L     |  0.8410 |  0.3060 |
| M     |  0.8050 |  0.2890 |
| N     |  0.8520 |  0.3010 |
| O     |  0.8790 |  0.2790 |
| P     |  0.9210 |  0.3330 |
| Q     |  0.9110 |  0.3460 |
| R     |  0.8730 |  0.2320 |
| S     |  0.9110 |  0.2370 |
| T     |  0.9310 |  0.2600 |
| V     |  0.8600 |  0.2450 |
| Y     |  0.9330 |  0.3310 |
| Z     |  0.8200 |  0.2690 |
| a     |  0.9170 |  0.3070 |
| b     |  0.8880 |  0.2390 |
| c     |  0.8820 |  0.2080 |



*Continued on next page...*

*Continued from previous page...*

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| d     |  0.9120   |  0.2490   |
| e     |  0.9020   |  0.2170   |
| f     |  0.9040   |  0.2210   |
| h     |  0.8870   |  0.2810   |
| i     |  0.8850   |  0.3160   |
| k     |  0.9600   |  0.2020   |
| m     |  0.8250   |  0.1530   |
| n     |  0.8240   |  0.2720   |
| o     |  0.8700   |  0.1880   |
| p     |  0.9040   |  0.3000   |
| q     |  0.8660   |  0.2420   |
| r     |  0.8270   |  0.1290   |
| s     |  0.8410   |  0.1650   |
| t     |  0.9630   |  0.1080   |
| u     |  0.7060   |  0.1010   |
| v     |  0.7540   |  0.0650   |
| w     |  0.9330   |  0.1920   |
| x     |  0.7950  |  0.1230  |
| y     |  0.7390 |  0.1240 |