



## Full wwPDB EM Validation Report ⓘ

Jun 25, 2026 – 12:36 AM EDT

PDB ID : 8VVR / pdb\_00008vvr  
EMDB ID : EMD-43566  
Title : Post-decoding/Post-hydrolysis state obtained from Anisomycin-treated mammalian ribosomes  
Authors : Loerch, S.; Petrossian, E.; Smith, P.R.; Campbell, Z.T.  
Deposited on : 2024-01-31  
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

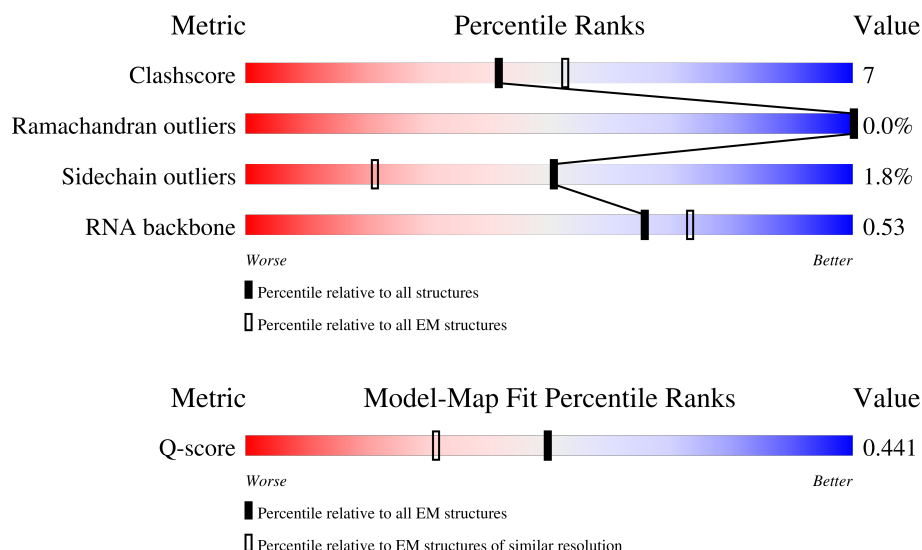
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01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

# 1 Overall quality at a glance

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

The reported resolution of this entry is 3.10 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                       | 14724 ( 2.60 - 3.60 )                                    |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 257    |                  |
| 2   | B     | 403    |                  |
| 3   | C     | 413    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 4   | D     | 297    |                  |
| 5   | E     | 291    |                  |
| 6   | F     | 249    |                  |
| 7   | G     | 319    |                  |
| 8   | H     | 192    |                  |
| 9   | I     | 214    |                  |
| 10  | J     | 178    |                  |
| 11  | K     | 211    |                  |
| 12  | L     | 218    |                  |
| 13  | M     | 204    |                  |
| 14  | N     | 203    |                  |
| 15  | O     | 213    |                  |
| 16  | P     | 188    |                  |
| 17  | Q     | 212    |                  |
| 18  | R     | 224    |                  |
| 19  | S     | 160    |                  |
| 20  | T     | 128    |                  |
| 21  | U     | 140    |                  |
| 22  | V     | 157    |                  |
| 23  | W     | 156    |                  |
| 24  | X     | 145    |                  |
| 25  | Y     | 136    |                  |
| 26  | Z     | 148    |                  |
| 27  | AA    | 245    |                  |
| 28  | BA    | 115    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 29  | CA    | 125    |                  |
| 30  | DA    | 135    |                  |
| 31  | EA    | 110    |                  |
| 32  | FA    | 129    |                  |
| 33  | GA    | 123    |                  |
| 34  | HA    | 105    |                  |
| 35  | IA    | 97     |                  |
| 36  | JA    | 70     |                  |
| 37  | KA    | 51     |                  |
| 38  | LA    | 128    |                  |
| 39  | MA    | 25     |                  |
| 40  | NA    | 106    |                  |
| 41  | OA    | 92     |                  |
| 42  | PA    | 137    |                  |
| 43  | RA    | 165    |                  |
| 44  | SA    | 76     |                  |
| 45  | TA    | 76     |                  |
| 46  | UA    | 75     |                  |
| 47  | VA    | 12     |                  |
| 48  | WA    | 3584   |                  |
| 49  | XA    | 120    |                  |
| 50  | YA    | 156    |                  |
| 51  | ZA    | 1869   |                  |
| 52  | AB    | 295    |                  |
| 53  | BB    | 264    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 54  | CB    | 293    |                  |
| 55  | DB    | 281    |                  |
| 56  | EB    | 263    |                  |
| 57  | FB    | 204    |                  |
| 58  | GB    | 249    |                  |
| 59  | HB    | 432    |                  |
| 60  | IB    | 208    |                  |
| 61  | JB    | 194    |                  |
| 62  | KB    | 165    |                  |
| 63  | LB    | 158    |                  |
| 64  | MB    | 132    |                  |
| 65  | NB    | 151    |                  |
| 66  | OB    | 151    |                  |
| 67  | PB    | 145    |                  |
| 68  | QB    | 172    |                  |
| 69  | RB    | 135    |                  |
| 70  | SB    | 152    |                  |
| 71  | TB    | 145    |                  |
| 72  | UB    | 119    |                  |
| 73  | VB    | 83     |                  |
| 74  | WB    | 130    |                  |
| 75  | XB    | 143    |                  |
| 76  | YB    | 131    |                  |
| 77  | ZB    | 124    |                  |
| 78  | AC    | 115    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 79  | BC    | 84     |                  |
| 80  | CC    | 69     |                  |
| 81  | DC    | 56     |                  |
| 82  | EC    | 133    |                  |
| 83  | FC    | 188    |                  |
| 84  | GC    | 317    |                  |
| 85  | IC    | 4      |                  |
| 86  | b     | 318    |                  |
| 87  | c     | 14     |                  |
| 88  | HC    | 462    |                  |

## 2 Entry composition

There are 95 unique types of molecules in this entry. The entry contains 220661 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 uL2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 1   | A     | 250      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1914  | 1199 | 392 | 317 | 6 |         |       |

- Molecule 2 is a protein called uL3.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 2   | B     | 397      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3196  | 2035 | 603 | 545 | 13 |         |       |

- Molecule 3 is a protein called uL4.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 3   | C     | 362      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2883  | 1812 | 577 | 480 | 14 |         |       |

- Molecule 4 is a protein called uL18.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 4   | D     | 294      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2395  | 1514 | 439 | 428 | 14 |         |       |

- Molecule 5 is a protein called L6.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 5   | E     | 228      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1823  | 1173 | 349 | 298 | 3 |         |       |

- Molecule 6 is a protein called uL30.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 6   | F     | 227      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1897  | 1217 | 366 | 305 | 9 |         |       |

- Molecule 7 is a protein called L7A.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 7   | G     | 229      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1850  | 1181 | 356 | 309 | 4 |         |       |

- Molecule 8 is a protein called L9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 8   | H     | 190      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1516  | 954 | 284 | 272 | 6 |         |       |

- Molecule 9 is a protein called L10.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 9   | I     | 205      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1664  | 1056 | 321 | 274 | 13 |         |       |

- Molecule 10 is a protein called uL5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 10  | J     | 171      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1372  | 867 | 256 | 243 | 6 |         |       |

- Molecule 11 is a protein called eL13.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 11  | K     | 210      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1702  | 1065 | 354 | 279 | 4 |         |       |

There are 9 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment   | Reference  |
|-------|---------|----------|--------|-----------|------------|
| K     | 46      | ILE      | -      | insertion | UNP G1TPV0 |
| K     | 47      | ALA      | -      | insertion | UNP G1TPV0 |
| K     | 48      | PRO      | -      | insertion | UNP G1TPV0 |
| K     | 49      | ARG      | -      | insertion | UNP G1TPV0 |
| K     | 50      | PRO      | -      | insertion | UNP G1TPV0 |
| K     | 51      | ALA      | -      | insertion | UNP G1TPV0 |
| K     | 52      | ALA      | -      | insertion | UNP G1TPV0 |
| K     | 53      | GLY      | -      | insertion | UNP G1TPV0 |
| K     | 54      | PRO      | -      | insertion | UNP G1TPV0 |

- Molecule 12 is a protein called eL14.



| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 12  | L     | 138      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1137  | 727 | 221 | 182 | 7 |         |       |

- Molecule 13 is a protein called eL15.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 13  | M     | 203      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1701  | 1072 | 359 | 266 | 4 |         |       |

- Molecule 14 is a protein called uL13.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 14  | N     | 199      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1630  | 1051 | 319 | 255 | 5 |         |       |

- Molecule 15 is a protein called uL22.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 15  | O     | 156      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1266  | 793 | 245 | 219 | 9 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| O     | 43      | SER      | ALA    | conflict | UNP G1TVT6 |

- Molecule 16 is a protein called eL18.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 16  | P     | 187      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1515  | 946 | 315 | 250 | 4 |         |       |

There are 12 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| P     | 4       | ASP      | ASN    | conflict | UNP G1TFE0 |
| P     | 14      | ARG      | TRP    | conflict | UNP G1TFE0 |
| P     | 53      | MET      | LEU    | conflict | UNP G1TFE0 |
| P     | 58      | ARG      | TRP    | conflict | UNP G1TFE0 |
| P     | 75      | ARG      | GLN    | conflict | UNP G1TFE0 |
| P     | 80      | ALA      | PRO    | conflict | UNP G1TFE0 |
| P     | 86      | VAL      | ILE    | conflict | UNP G1TFE0 |

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| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| P     | 104     | ARG      | HIS    | conflict | UNP G1TFE0 |
| P     | 110     | ARG      | CYS    | conflict | UNP G1TFE0 |
| P     | 137     | VAL      | GLY    | conflict | UNP G1TFE0 |
| P     | 157     | GLY      | ARG    | conflict | UNP G1TFE0 |
| P     | 181     | ARG      | TRP    | conflict | UNP G1TFE0 |

- Molecule 17 is a protein called eL19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 17  | Q     | 180      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1508  | 933 | 328 | 238 | 9 |         |       |

- Molecule 18 is a protein called eL20.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 18  | R     | 176      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1462  | 930 | 285 | 236 | 11 |         |       |

- Molecule 19 is a protein called eL21.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19  | S     | 159      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1298  | 823 | 252 | 217 | 6 |         |       |

- Molecule 20 is a protein called eL22.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 20  | T     | 101      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 826   | 530 | 144 | 150 | 2 |         |       |

There are 11 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| T     | 18      | LEU      | VAL    | conflict | UNP G1TSG1 |
| T     | 32      | GLY      | ARG    | conflict | UNP G1TSG1 |
| T     | 36      | ALA      | GLU    | conflict | UNP G1TSG1 |
| T     | 39      | PHE      | SER    | conflict | UNP G1TSG1 |
| T     | 54      | GLY      | ARG    | conflict | UNP G1TSG1 |
| T     | 60      | VAL      | ALA    | conflict | UNP G1TSG1 |
| T     | 62      | SER      | THR    | conflict | UNP G1TSG1 |
| T     | 63      | LEU      | ILE    | conflict | UNP G1TSG1 |

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| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| T     | 97      | ARG      | HIS    | conflict | UNP G1TSG1 |
| T     | 106     | THR      | SER    | conflict | UNP G1TSG1 |
| T     | 126     | GLU      | ASP    | conflict | UNP G1TSG1 |

- Molecule 21 is a protein called L23.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 21  | U     | 135      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1004  | 631 | 191 | 177 | 5 |         |       |

- Molecule 22 is a protein called uL24.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 22  | V     | 110      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 887   | 555 | 179 | 149 | 4 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| V     | 78      | SER      | PHE    | conflict | UNP G1SE28 |

- Molecule 23 is a protein called uL23.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 23  | W     | 118      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 967   | 618 | 181 | 167 | 1 |         |       |

- Molecule 24 is a protein called L26.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 24  | X     | 134      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1115  | 700 | 226 | 186 | 3 |         |       |

- Molecule 25 is a protein called L27.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 25  | Y     | 135      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1107  | 714 | 208 | 182 | 3 |         |       |

- Molecule 26 is a protein called uL15.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 26  | Z     | 147      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1162  | 734 | 239 | 185 | 4 |         |       |

- Molecule 27 is a protein called L29.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 27  | AA    | 107      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 873   | 542 | 195 | 133 | 3 |         |       |

- Molecule 28 is a protein called eL30.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 28  | BA    | 99       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 769   | 486 | 135 | 141 | 7 |         |       |

- Molecule 29 is a protein called L31.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 29  | CA    | 108      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 893   | 563 | 172 | 156 | 2 |         |       |

- Molecule 30 is a protein called L32.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 30  | DA    | 129      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1064  | 673 | 220 | 166 | 5 |         |       |

- Molecule 31 is a protein called eL33.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 31  | EA    | 109      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 876   | 555 | 174 | 143 | 4 |         |       |

- Molecule 32 is a protein called L34.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 32  | FA    | 114      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 906   | 566 | 187 | 147 | 6 |         |       |

- Molecule 33 is a protein called L35.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 33  | GA    | 121      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1008  | 637 | 203 | 167 | 1 |         |       |

- Molecule 34 is a protein called L36.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 34  | HA    | 102      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 830   | 520 | 176 | 129 | 5 |         |       |

- Molecule 35 is a protein called L37.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 35  | IA    | 87       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 716   | 440 | 159 | 112 | 5 |         |       |

- Molecule 36 is a protein called eL38.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 36  | JA    | 69       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 569   | 366 | 103 | 99 | 1 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| JA    | 24      | LYS      | ASN    | conflict | UNP G1U001 |

- Molecule 37 is a protein called eL39.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 37  | KA    | 50       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 447   | 286 | 96 | 64 | 1 |         |       |

- Molecule 38 is a protein called eL40.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 38  | LA    | 52       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 429   | 266 | 90 | 67 | 6 |         |       |

- Molecule 39 is a protein called eL41.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 39  | MA    | 25       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 239   | 145 | 64 | 27 | 3 |         |       |

- Molecule 40 is a protein called eL42.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 40  | NA    | 104      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 851   | 533 | 174 | 138 | 6 |         |       |

- Molecule 41 is a protein called eL43.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 41  | OA    | 91       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 708   | 445 | 136 | 120 | 7 |         |       |

- Molecule 42 is a protein called L28.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 42  | PA    | 124      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 994   | 616 | 205 | 167 | 6 |         |       |

- Molecule 43 is a protein called L12.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 43  | RA    | 153      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1160  | 722 | 218 | 217 | 3 |         |       |

- Molecule 44 is a RNA chain called P-site tRNA.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 44  | SA    | 76       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1622  | 726 | 300 | 521 | 75 |         |       |

- Molecule 45 is a RNA chain called E-site tRNA.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 45  | TA    | 76       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1615  | 722 | 286 | 532 | 75 |         |       |

- Molecule 46 is a RNA chain called A-site tRNA.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 46  | UA    | 75       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1596  | 713 | 285 | 523 | 75 |         |       |

- Molecule 47 is a RNA chain called mRNA.

| Mol | Chain | Residues | Atoms |     |    |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|----|---------|-------|
| 47  | VA    | 12       | Total | C   | N  | O  | P  | 0       | 0     |
|     |       |          | 251   | 113 | 41 | 85 | 12 |         |       |

- Molecule 48 is a RNA chain called 28S rRNA.

| Mol | Chain | Residues | Atoms |       |       |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|-------|
| 48  | WA    | 3578     | Total | C     | N     | O     | P    | 0       | 0     |
|     |       |          | 76735 | 34173 | 14061 | 24923 | 3578 |         |       |

- Molecule 49 is a RNA chain called 5S rRNA.

| Mol | Chain | Residues | Atoms |      |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
| 49  | XA    | 119      | Total | C    | N   | O   | P   | 0       | 0     |
|     |       |          | 2538  | 1132 | 454 | 834 | 118 |         |       |

There are 7 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference   |
|-------|---------|----------|--------|----------|-------------|
| XA    | 2       | U        | N      | conflict | GB X06789.1 |
| XA    | 36      | C        | N      | conflict | GB X06789.1 |
| XA    | 102     | U        | N      | conflict | GB X06789.1 |
| XA    | 112     | U        | N      | conflict | GB X06789.1 |
| XA    | 114     | U        | N      | conflict | GB X06789.1 |
| XA    | 119     | U        | C      | conflict | GB X06789.1 |
| XA    | 120     | U        | N      | conflict | GB X06789.1 |

- Molecule 50 is a RNA chain called 5.8S rRNA.

| Mol | Chain | Residues | Atoms |      |     |      |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|-----|---------|-------|
| 50  | YA    | 156      | Total | C    | N   | O    | P   | 0       | 0     |
|     |       |          | 3314  | 1480 | 585 | 1094 | 155 |         |       |

- Molecule 51 is a RNA chain called 18S rRNA.

| Mol | Chain | Residues | Atoms |       |      |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|-------|
| 51  | ZA    | 1716     | Total | C     | N    | O     | P    | 0       | 0     |
|     |       |          | 36623 | 16347 | 6572 | 11989 | 1715 |         |       |

- Molecule 52 is a protein called RPSA.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 52  | AB    | 217      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1710  | 1086 | 300 | 316 | 8 |         |       |

- Molecule 53 is a protein called S3A.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 53  | BB    | 213      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1729  | 1098 | 309 | 308 | 14 |         |       |

- Molecule 54 is a protein called eS1.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 54  | CB    | 220      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1707  | 1105 | 293 | 300 | 9 |         |       |

- Molecule 55 is a protein called S3.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 55  | DB    | 228      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1768  | 1126 | 318 | 316 | 8 |         |       |

- Molecule 56 is a protein called S4.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 56  | EB    | 262      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2076  | 1324 | 386 | 358 | 8 |         |       |

There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| EB    | 25      | GLY      | SER    | conflict | UNP G1TK17 |
| EB    | 51      | ARG      | LYS    | conflict | UNP G1TK17 |
| EB    | 78      | THR      | ALA    | conflict | UNP G1TK17 |
| EB    | 156     | VAL      | MET    | conflict | UNP G1TK17 |

- Molecule 57 is a protein called S5.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 57  | FB    | 185      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1471  | 921 | 277 | 266 | 7 |         |       |



- Molecule 58 is a protein called eS6.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 58  | GB    | 237      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1923  | 1200 | 387 | 329 | 7 |         |       |

- Molecule 59 is a protein called eS7.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 59  | HB    | 185      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1489  | 952 | 271 | 265 | 1 |         |       |

- Molecule 60 is a protein called S8.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 60  | IB    | 206      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1686  | 1058 | 332 | 291 | 5 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| IB    | 47      | ARG      | GLY    | conflict | UNP G1TJW1 |

- Molecule 61 is a protein called S9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 61  | JB    | 185      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1525  | 969 | 306 | 248 | 2 |         |       |

- Molecule 62 is a protein called S10.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 62  | KB    | 96       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 810   | 530 | 143 | 131 | 6 |         |       |

- Molecule 63 is a protein called S11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 63  | LB    | 144      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1180  | 752 | 223 | 199 | 6 |         |       |

- Molecule 64 is a protein called S12.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 64  | MB    | 117      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 908   | 570 | 161 | 169 | 8 |         |       |

- Molecule 65 is a protein called uS15.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 65  | NB    | 149      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1202  | 770 | 228 | 203 | 1 |         |       |

- Molecule 66 is a protein called S14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 66  | OB    | 136      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1016  | 621 | 199 | 190 | 6 |         |       |

- Molecule 67 is a protein called S15.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 67  | PB    | 129      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1058  | 670 | 201 | 180 | 7 |         |       |

- Molecule 68 is a protein called uS9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 68  | QB    | 142      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1128  | 717 | 213 | 195 | 3 |         |       |

- Molecule 69 is a protein called eS17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 69  | RB    | 132      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1068  | 670 | 199 | 195 | 4 |         |       |

- Molecule 70 is a protein called S18.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 70  | SB    | 144      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1190  | 746 | 241 | 202 | 1 |         |       |

- Molecule 71 is a protein called S19.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 71  | TB    | 142      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1104  | 693 | 212 | 196 | 3 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| TB    | 119     | GLY      | TRP    | conflict | UNP G1TN62 |

- Molecule 72 is a protein called uS10.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 72  | UB    | 102      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 808   | 507 | 154 | 143 | 4 |         |       |

- Molecule 73 is a protein called S21.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 73  | VB    | 83       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 636   | 393 | 117 | 121 | 5 |         |       |

There are 7 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| VB    | 3       | ASN      | SER    | conflict | UNP G1TM82 |
| VB    | 4       | ASP      | ASN    | conflict | UNP G1TM82 |
| VB    | 33      | GLN      | PRO    | conflict | UNP G1TM82 |
| VB    | 50      | PHE      | SER    | conflict | UNP G1TM82 |
| VB    | 75      | ALA      | SER    | conflict | UNP G1TM82 |
| VB    | 76      | ASP      | HIS    | conflict | UNP G1TM82 |
| VB    | 81      | LYS      | GLN    | conflict | UNP G1TM82 |

- Molecule 74 is a protein called S15A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 74  | WB    | 129      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1034  | 659 | 193 | 176 | 6 |         |       |

- Molecule 75 is a protein called S23.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 75  | XB    | 141      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1098  | 693 | 219 | 183 | 3 |         |       |

- Molecule 76 is a protein called S24.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 76  | YB    | 124      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1011  | 640 | 198 | 168 | 5 |         |       |

- Molecule 77 is a protein called eS25.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 77  | ZB    | 85       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 683   | 439 | 128 | 115 | 1 |         |       |

- Molecule 78 is a protein called S26.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 78  | AC    | 101      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 814   | 507 | 170 | 132 | 5 |         |       |

There are 3 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| AC    | 28      | ARG      | CYS    | conflict | UNP G1TFE8 |
| AC    | 56      | ALA      | VAL    | conflict | UNP G1TFE8 |
| AC    | 109     | ARG      | PRO    | conflict | UNP G1TFE8 |

- Molecule 79 is a protein called S27.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 79  | BC    | 83       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 651   | 408 | 121 | 115 | 7 |         |       |

- Molecule 80 is a protein called S28.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 80  | CC    | 62       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 488   | 297 | 97 | 92 | 2 |         |       |

- Molecule 81 is a protein called uS14.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 81  | DC    | 55       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 459   | 286 | 94 | 74 | 5 |         |       |

- Molecule 82 is a protein called S30.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 82  | EC    | 55       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 443   | 274 | 97 | 71 | 1 |         |       |

- Molecule 83 is a protein called S27A.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 83  | FC    | 69       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 564   | 357 | 105 | 95 | 7 |         |       |

- Molecule 84 is a protein called RACK1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 84  | GC    | 313      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2436  | 1535 | 424 | 465 | 12 |         |       |

- Molecule 85 is a protein called peptide.

| Mol | Chain | Residues | Atoms |    |   |   | AltConf | Trace |
|-----|-------|----------|-------|----|---|---|---------|-------|
| 85  | IC    | 4        | Total | C  | N | O | 0       | 0     |
|     |       |          | 20    | 12 | 4 | 4 |         |       |

- Molecule 86 is a protein called RPLP0.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 86  | b     | 167      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1279  | 813 | 228 | 229 | 9 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| b     | 82      | LEU      | ILE    | conflict | UNP G1SPK4 |

- Molecule 87 is a protein called RPLP peptide.

| Mol | Chain | Residues | Atoms |    |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|-------|
| 87  | c     | 14       | Total | C  | N  | O  | S | 0       | 0     |
|     |       |          | 110   | 66 | 14 | 29 | 1 |         |       |

- Molecule 88 is a protein called eukaryotic elongation factor 1A.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 88  | HC    | 223      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1664  | 1048 | 299 | 308 | 9 |         |       |

- Molecule 89 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |     | AltConf |
|-----|-------|----------|-------|-----|---------|
| 89  | A     | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 89  | I     | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 89  | O     | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 89  | P     | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 89  | U     | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 89  | Z     | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 89  | FA    | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 89  | IA    | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 89  | VA    | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 89  | WA    | 142      | Total | Mg  | 0       |
|     |       |          | 142   | 142 |         |
| 89  | XA    | 4        | Total | Mg  | 0       |
|     |       |          | 4     | 4   |         |
| 89  | YA    | 2        | Total | Mg  | 0       |
|     |       |          | 2     | 2   |         |
| 89  | ZA    | 45       | Total | Mg  | 0       |
|     |       |          | 45    | 45  |         |
| 89  | AC    | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 89  | HC    | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |

- Molecule 90 is ZINC ION (CCD ID: ZN) (formula: Zn).

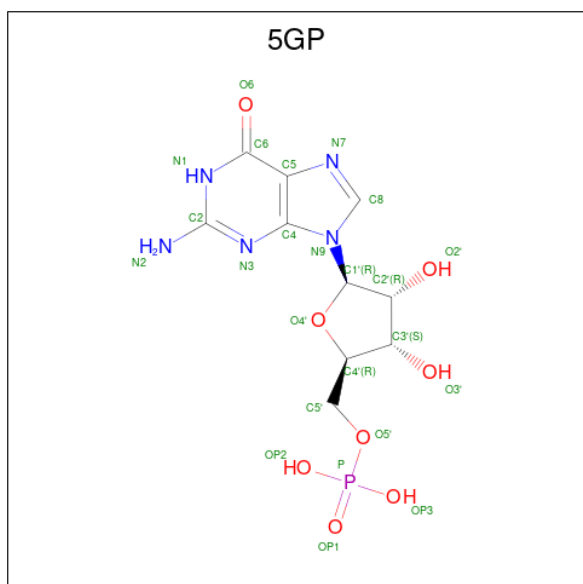
| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 90  | FA    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 90  | IA    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |

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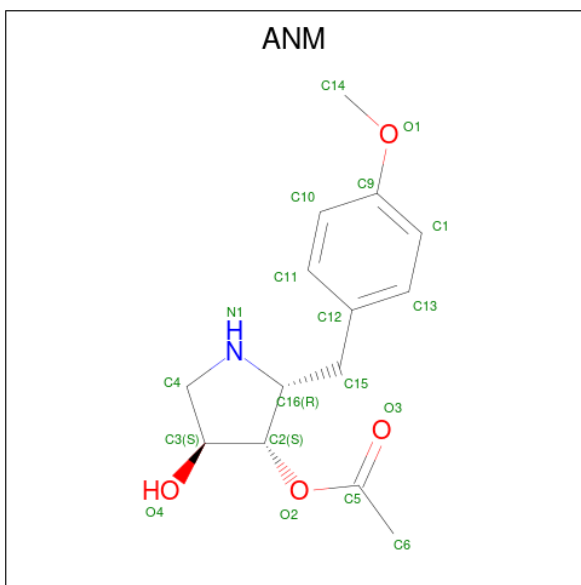
| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 90  | LA    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 90  | NA    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 90  | OA    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 90  | AC    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 90  | DC    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |
| 90  | FC    | 1        | Total | Zn | 0       |
|     |       |          | 1     | 1  |         |

- Molecule 91 is GUANOSINE-5'-MONOPHOSPHATE (CCD ID: 5GP) (formula:  $C_{10}H_{14}N_5O_8P$ ).



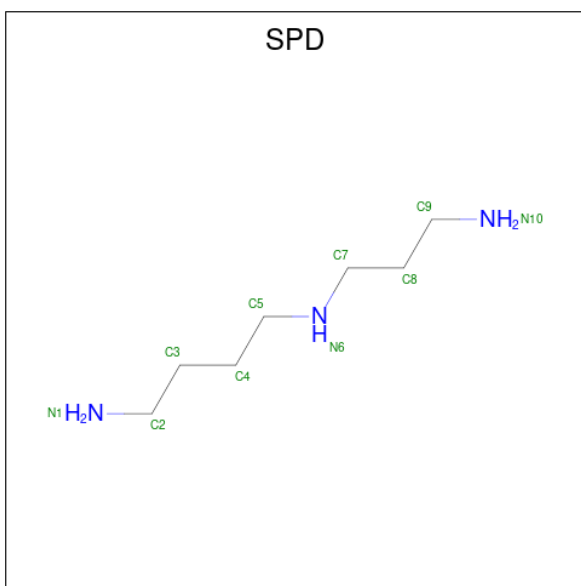
| Mol | Chain | Residues | Atoms |    |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 91  | UA    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 24    | 10 | 5 | 8 | 1 |         |

- Molecule 92 is ANISOMYCIN (CCD ID: ANM) (formula:  $C_{14}H_{19}NO_4$ ).



| Mol | Chain | Residues | Atoms |    |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---------|
| 92  | WA    | 1        | Total | C  | N | O | 0       |
|     |       |          | 19    | 14 | 1 | 4 |         |

- Molecule 93 is SPERMIDINE (CCD ID: SPD) (formula:  $C_7H_{19}N_3$ ).



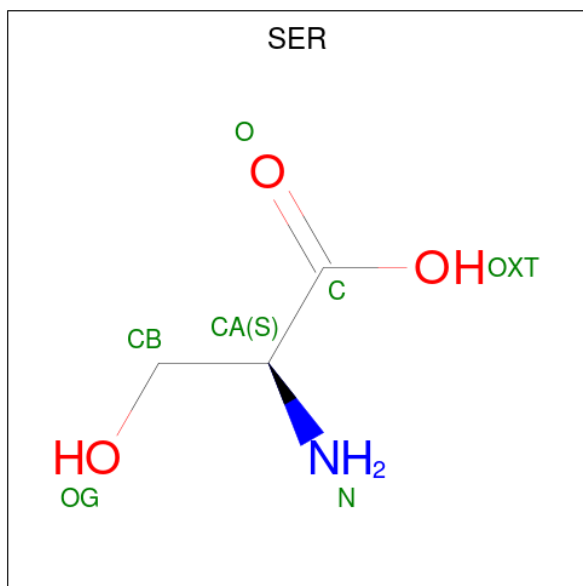
| Mol | Chain | Residues | Atoms |   |   | AltConf |
|-----|-------|----------|-------|---|---|---------|
| 93  | WA    | 1        | Total | C | N | 0       |
|     |       |          | 10    | 7 | 3 |         |
| 93  | WA    | 1        | Total | C | N | 0       |
|     |       |          | 10    | 7 | 3 |         |
| 93  | ZA    | 1        | Total | C | N | 0       |
|     |       |          | 10    | 7 | 3 |         |



- Molecule 94 is POTASSIUM ION (CCD ID: K) (formula: K).

| Mol | Chain | Residues | Atoms |   |  | AltConf |
|-----|-------|----------|-------|---|--|---------|
| 94  | WA    | 1        | Total | K |  | 0       |
|     |       |          | 1     | 1 |  |         |

- Molecule 95 is SERINE (CCD ID: SER) (formula: C<sub>3</sub>H<sub>7</sub>NO<sub>3</sub>).



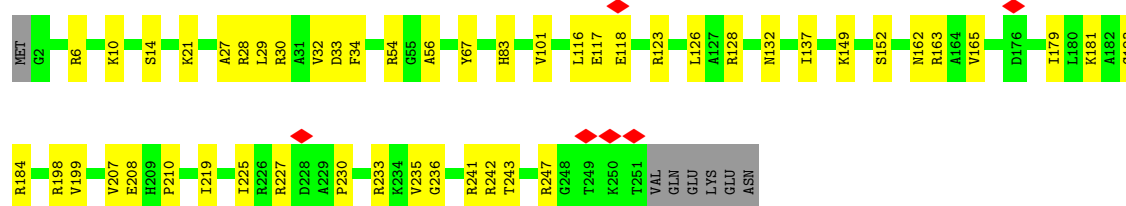
| Mol | Chain | Residues | Atoms |   |   |   | AltConf |
|-----|-------|----------|-------|---|---|---|---------|
| 95  | HC    | 1        | Total | C | N | O | 0       |
|     |       |          | 6     | 3 | 1 | 2 |         |

### 3 Residue-property plots [i](#)

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.

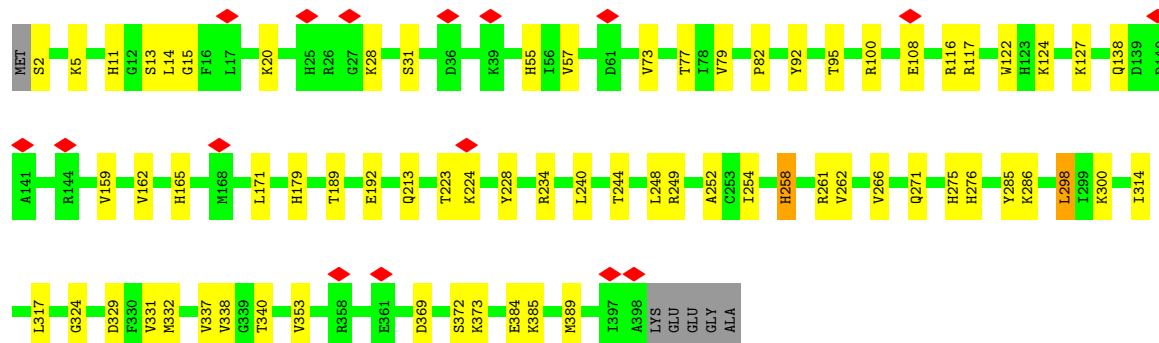
#### • Molecule 1: uL2

Chain A: 



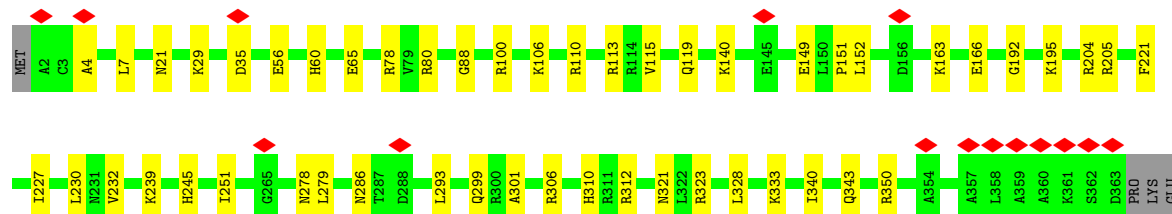
#### • Molecule 2: uL3

Chain B: 



#### • Molecule 3: uL4

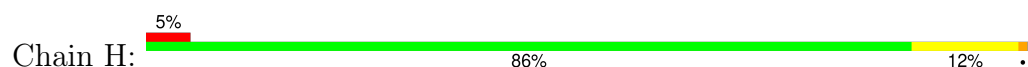
Chain C: 



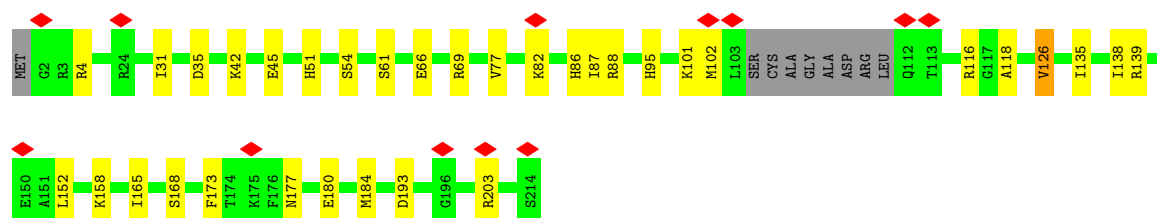
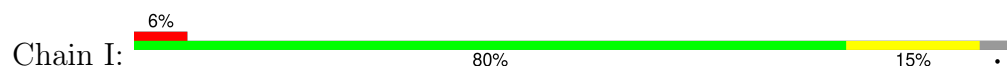
|     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| SER | GLU | GLN | LEU | PRO | THR | CYS | SER | SER | THR | THR | HIS | HIS | ASP | PHE | THR | THR | ASP | ASP | LYS | LYS | V80 | K90 | I94 | G95 | Q96 | D97 | I98 | R106 | P111 | I114 | R115 | Q119 | R126 | Q138 | V139 | R156 | P157 | E158 | T159 | E162 | R166 | R170 | A171 | E172 | K173 | K174 | A175 | A176 |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|



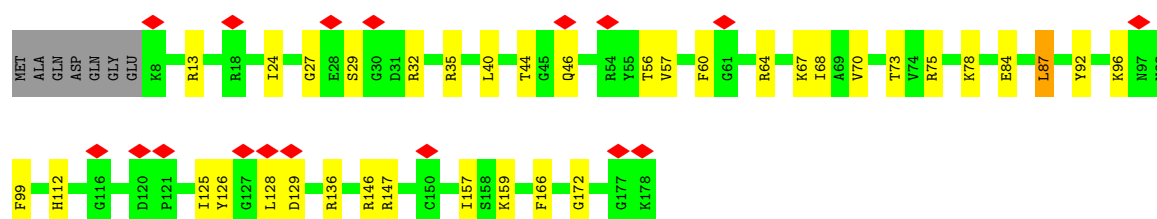
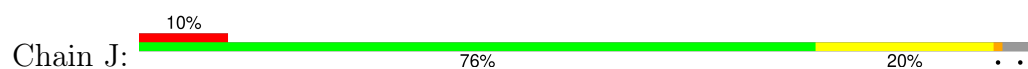
• Molecule 8: L9



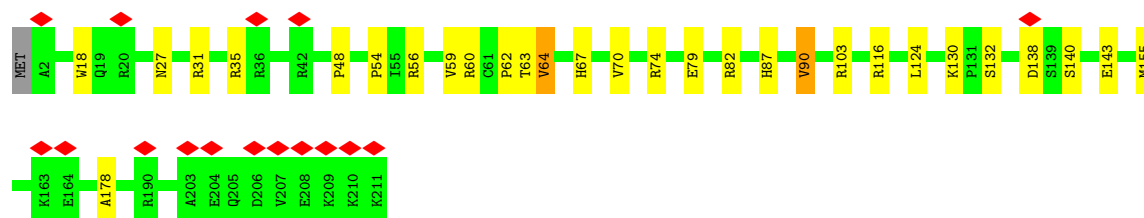
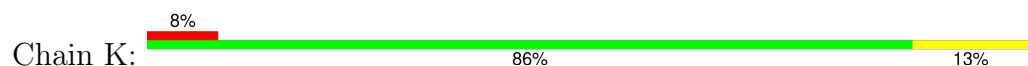
• Molecule 9: L10



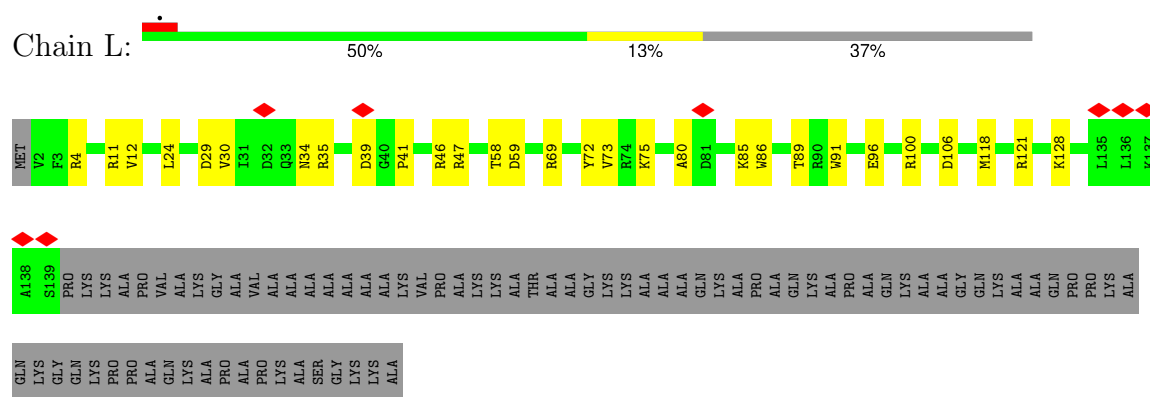
• Molecule 10: uL5



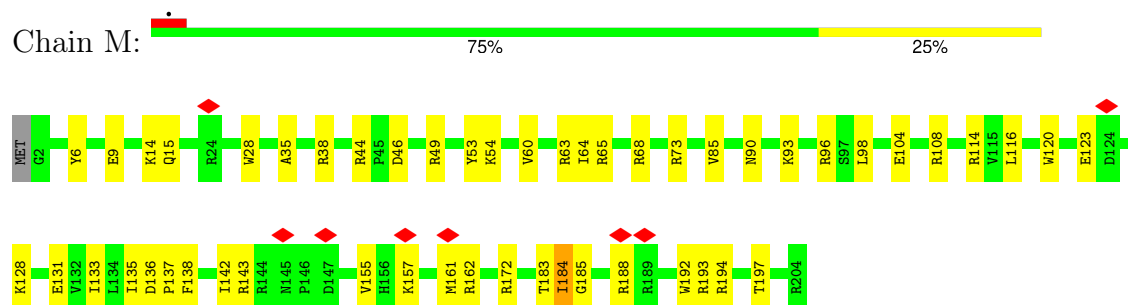
• Molecule 11: eL13



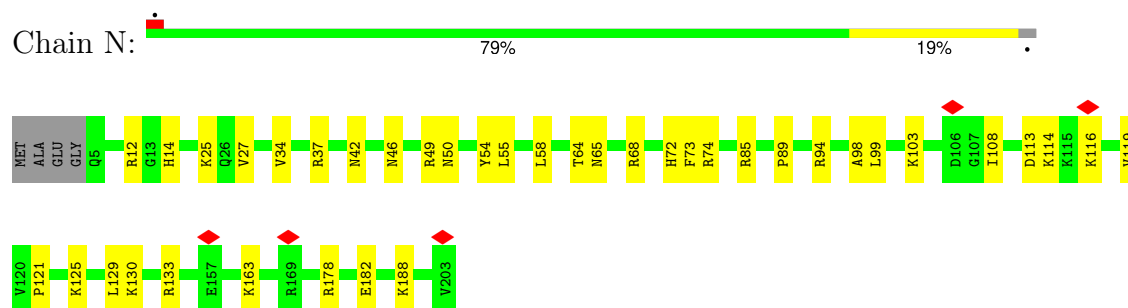
• Molecule 12: eL14



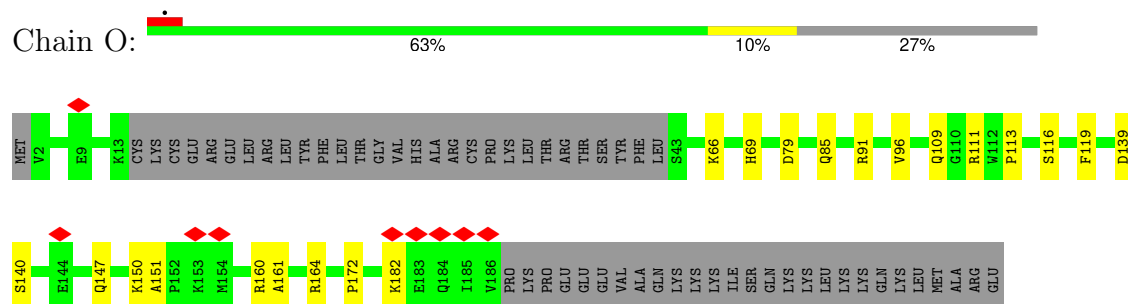
- Molecule 13: eL15



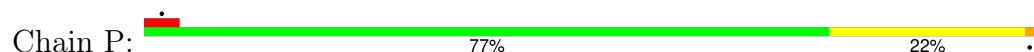
- Molecule 14: uL13

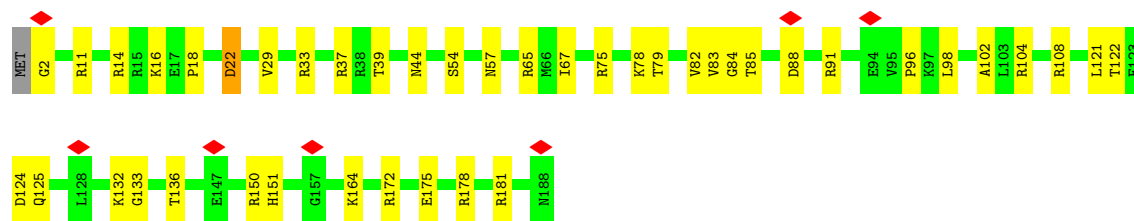


- Molecule 15: uL22

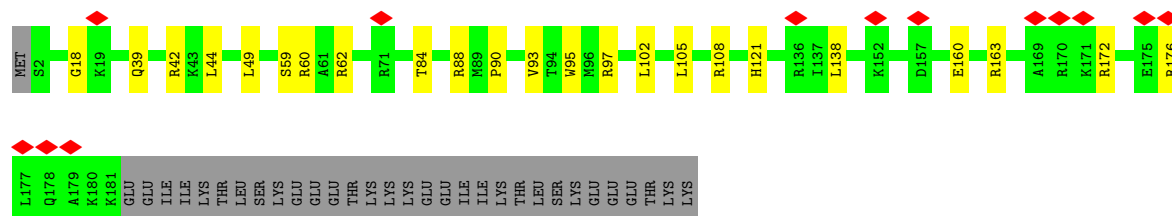
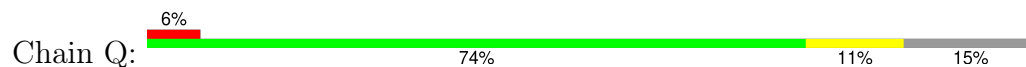


- Molecule 16: eL18

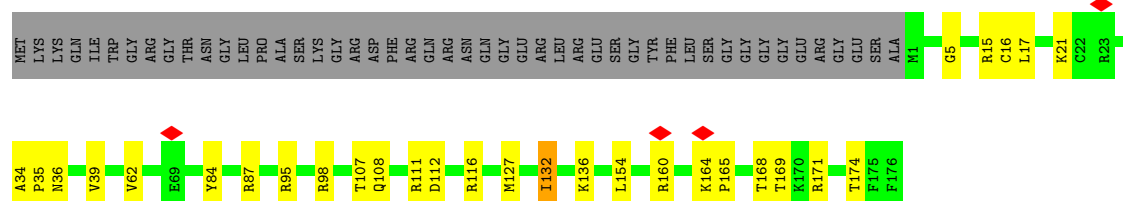




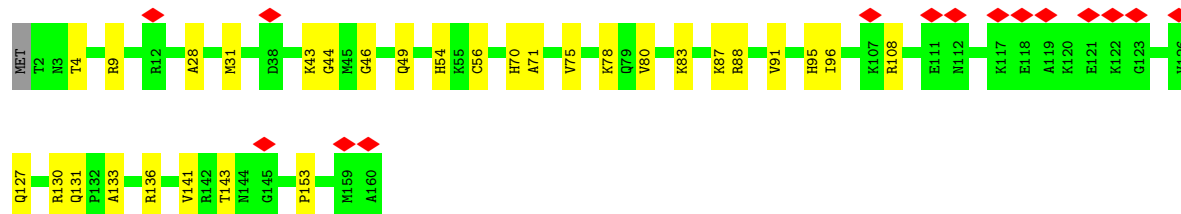
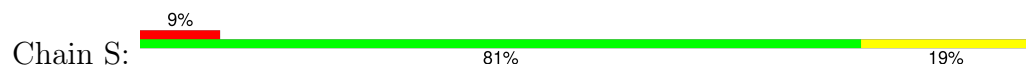
• Molecule 17: eL19



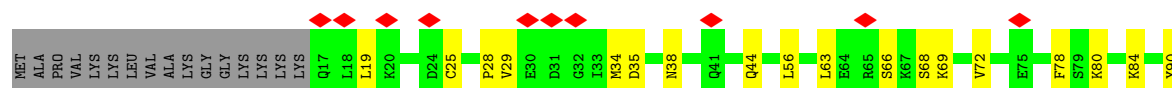
• Molecule 18: eL20



• Molecule 19: eL21

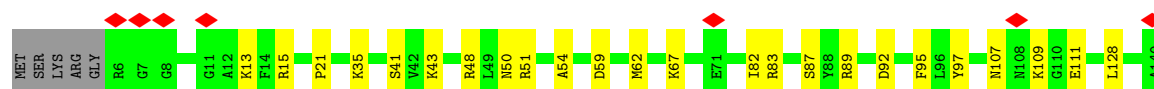
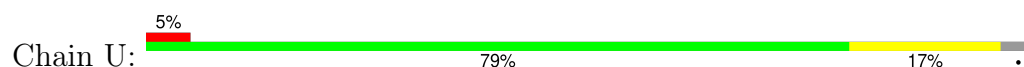


• Molecule 20: eL22

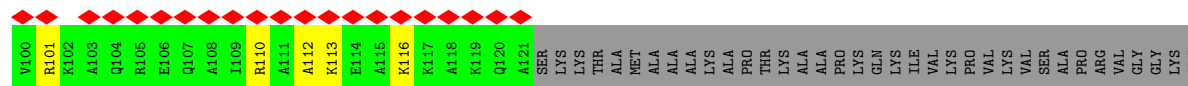
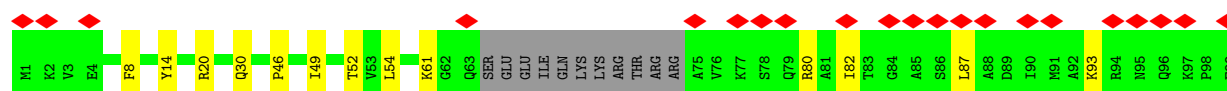




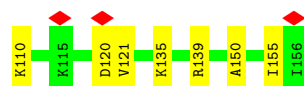
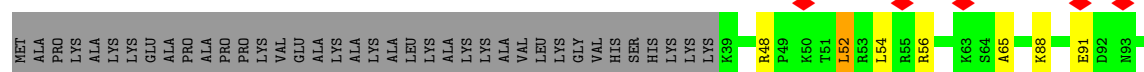
- Molecule 21: L23



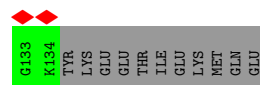
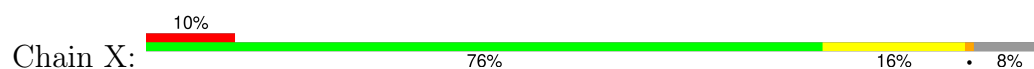
- Molecule 22: uL24



- Molecule 23: uL23

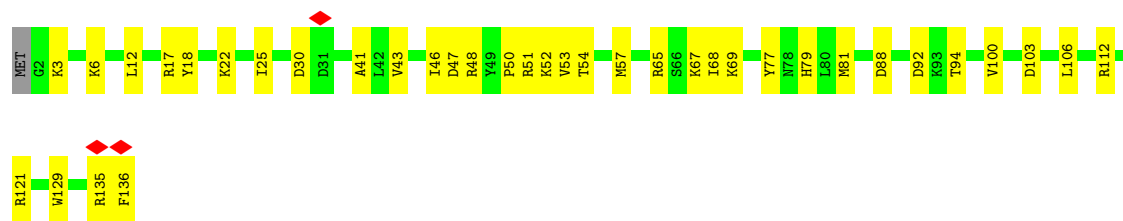


- Molecule 24: L26

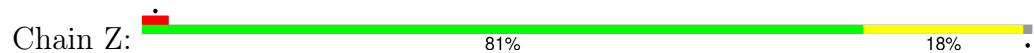


- Molecule 25: L27

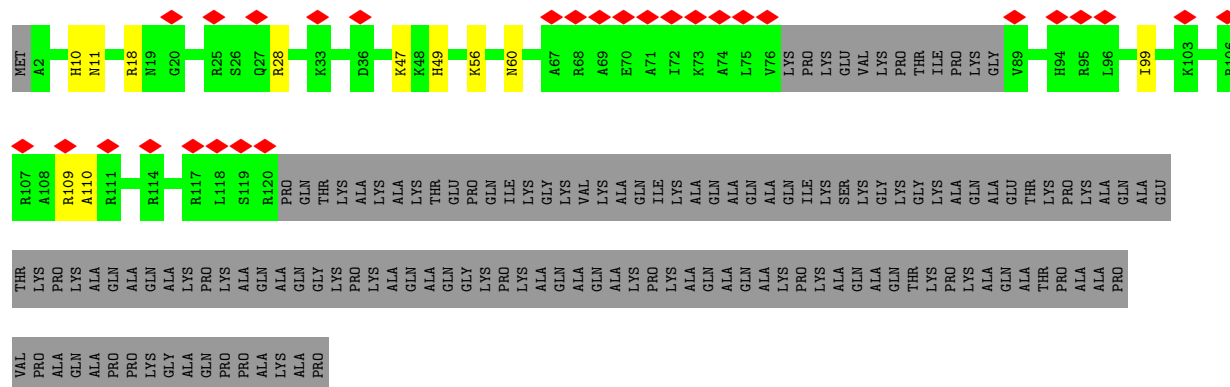
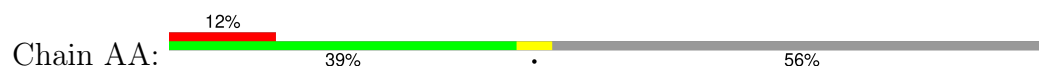




- Molecule 26: uL15



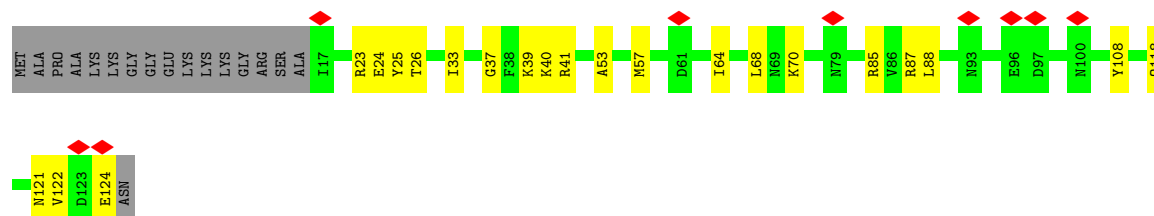
- Molecule 27: L29



- Molecule 28: eL30



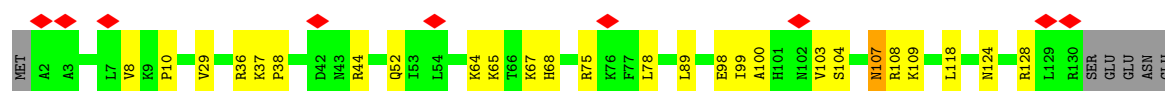
- Molecule 29: L31



- Molecule 30: L32



Chain DA: 



• Molecule 31: eL33

Chain EA: 



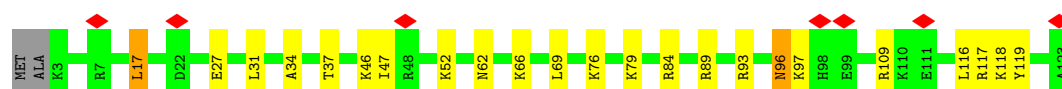
• Molecule 32: L34

Chain FA: 



• Molecule 33: L35

Chain GA: 



• Molecule 34: L36

Chain HA: 



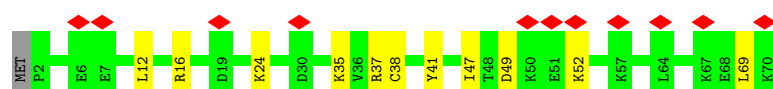
• Molecule 35: L37

Chain IA: 

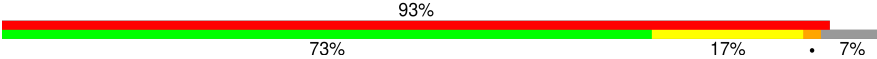


• Molecule 36: eL38

Chain JA: 



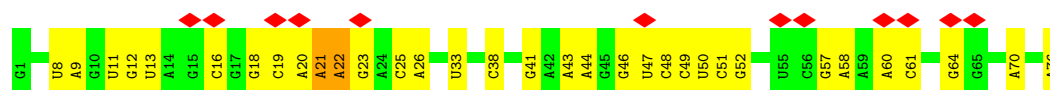


Chain RA: 



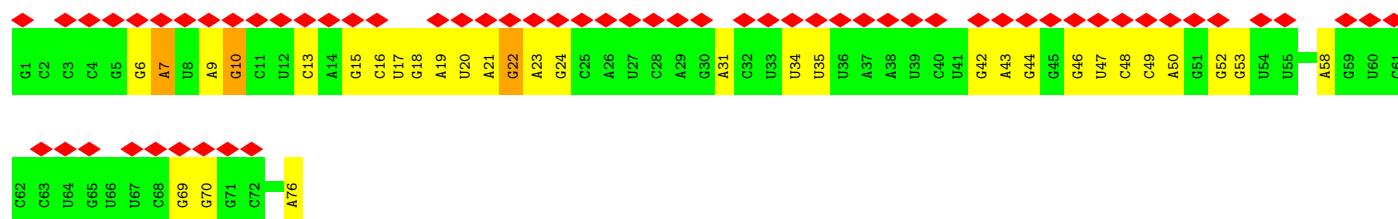
• Molecule 44: P-site tRNA

Chain SA: 



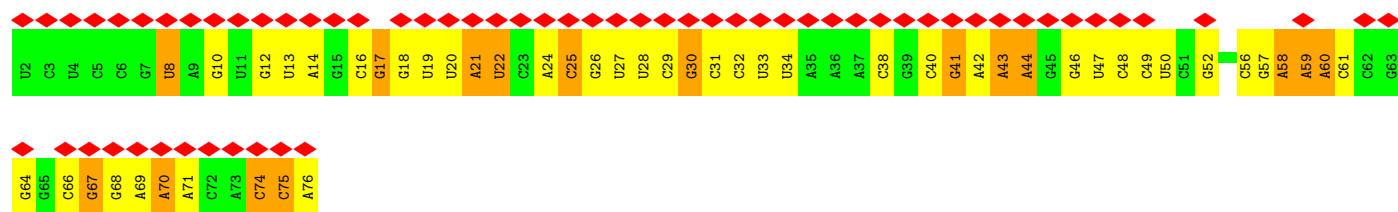
• Molecule 45: E-site tRNA

Chain TA: 



• Molecule 46: A-site tRNA

Chain UA: 

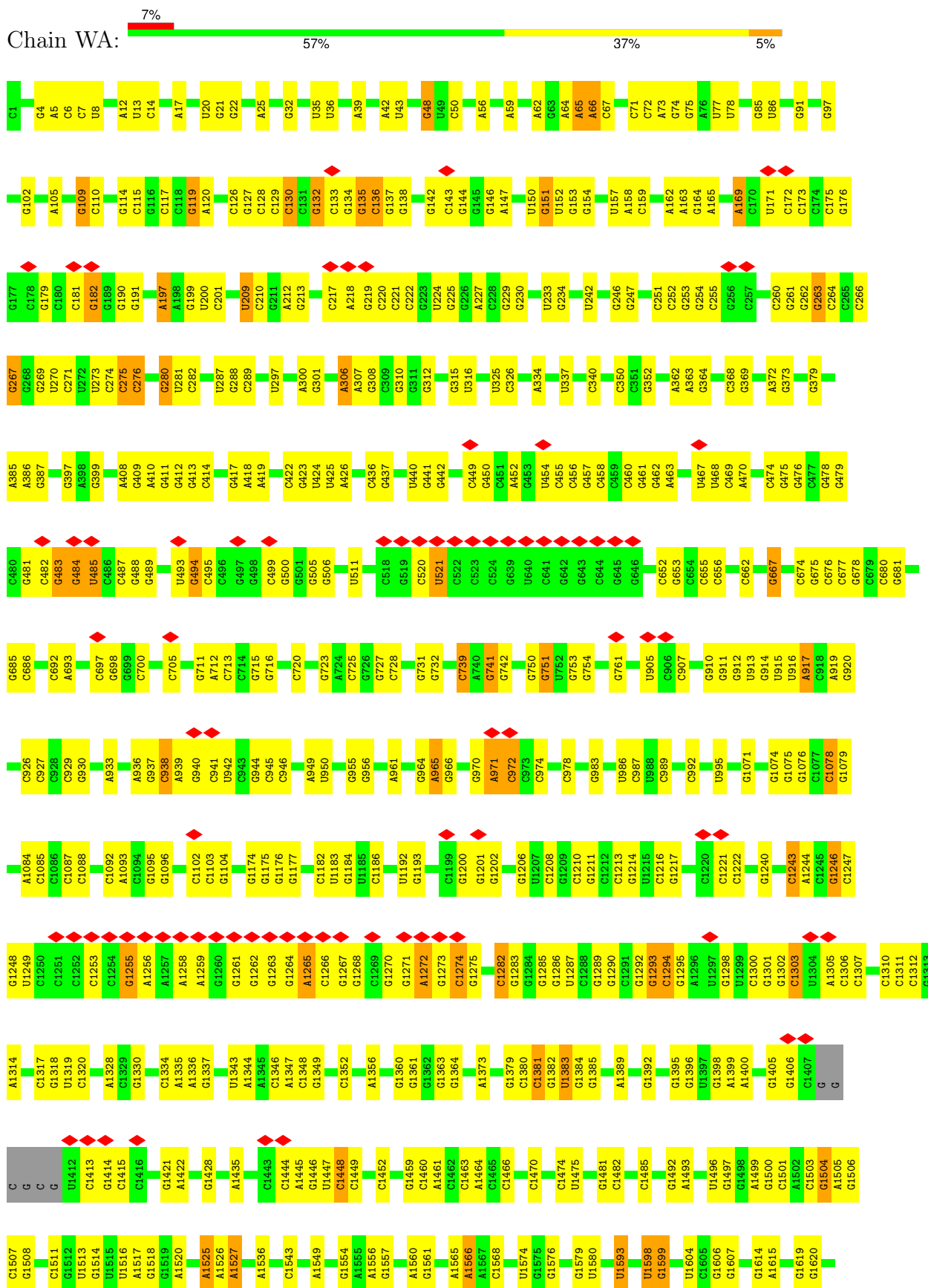


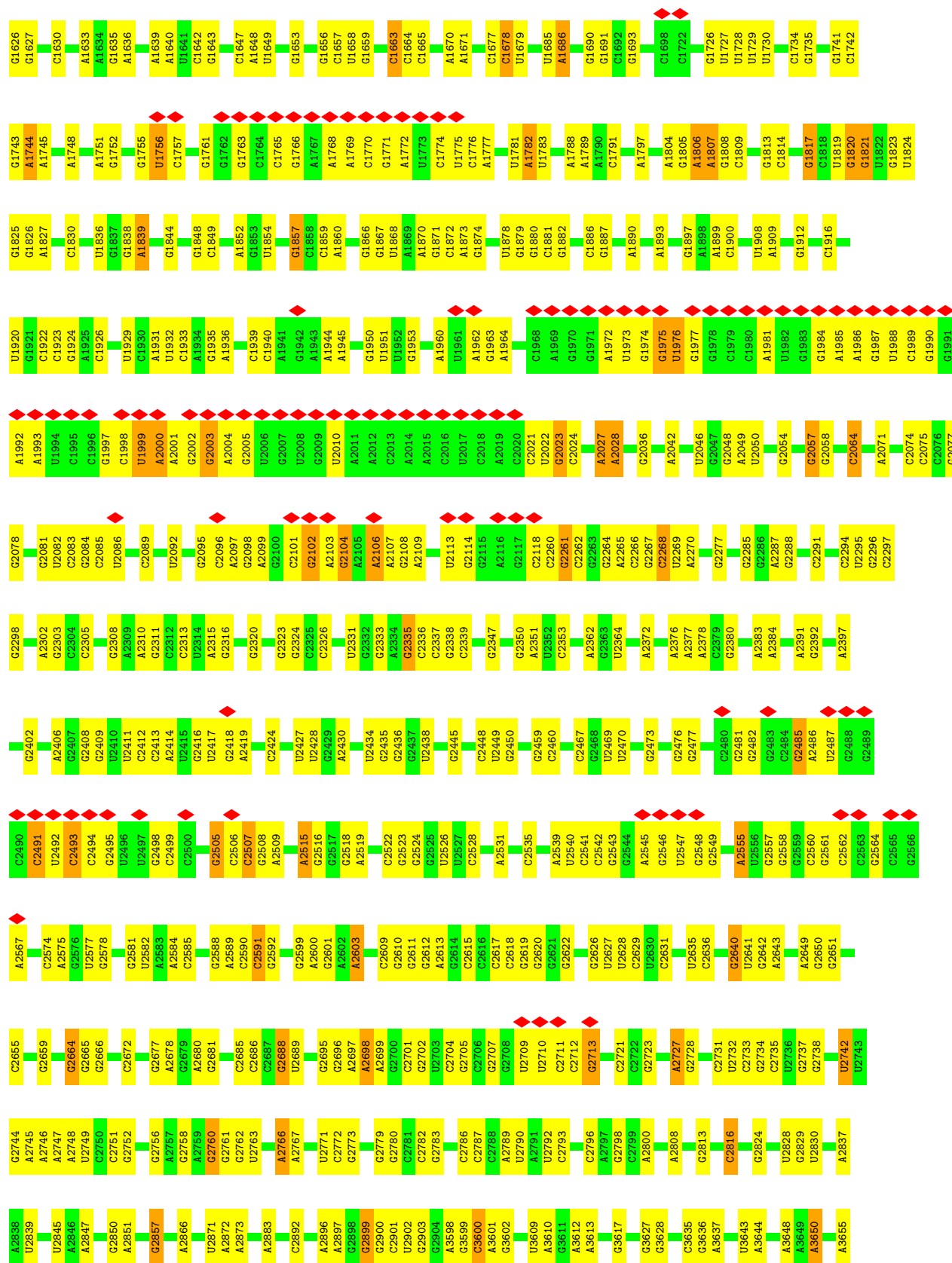
• Molecule 47: mRNA

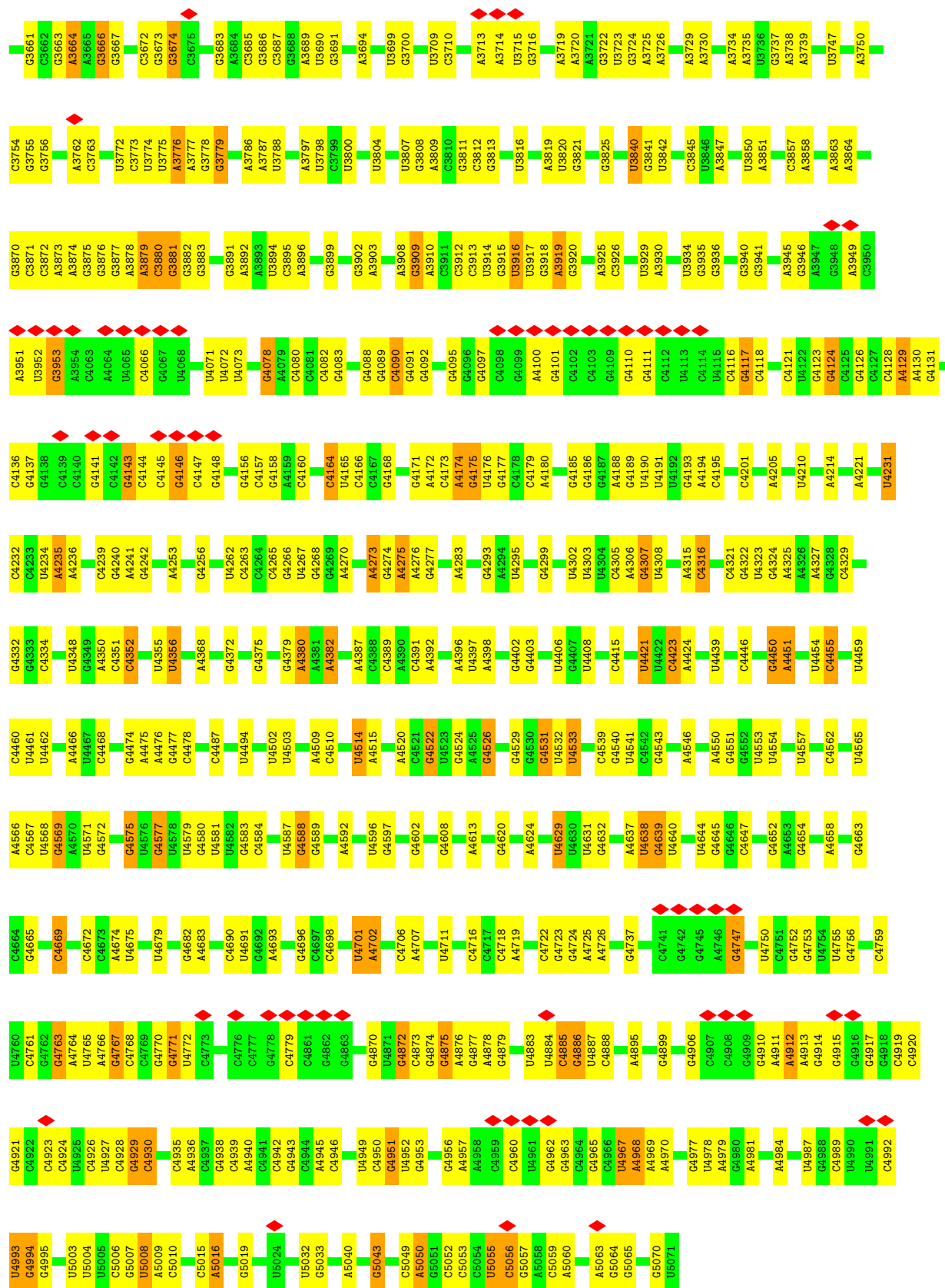
Chain VA: 



• Molecule 48: 28S rRNA







• Molecule 49: 5S rRNA

Chain XA: 



U

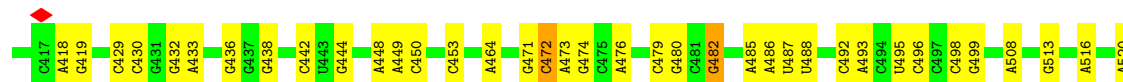
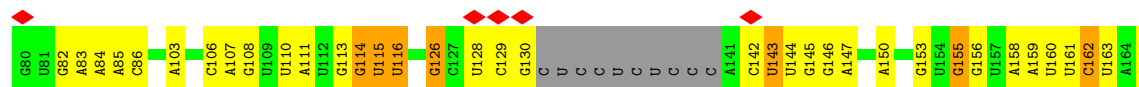
• Molecule 50: 5.8S rRNA

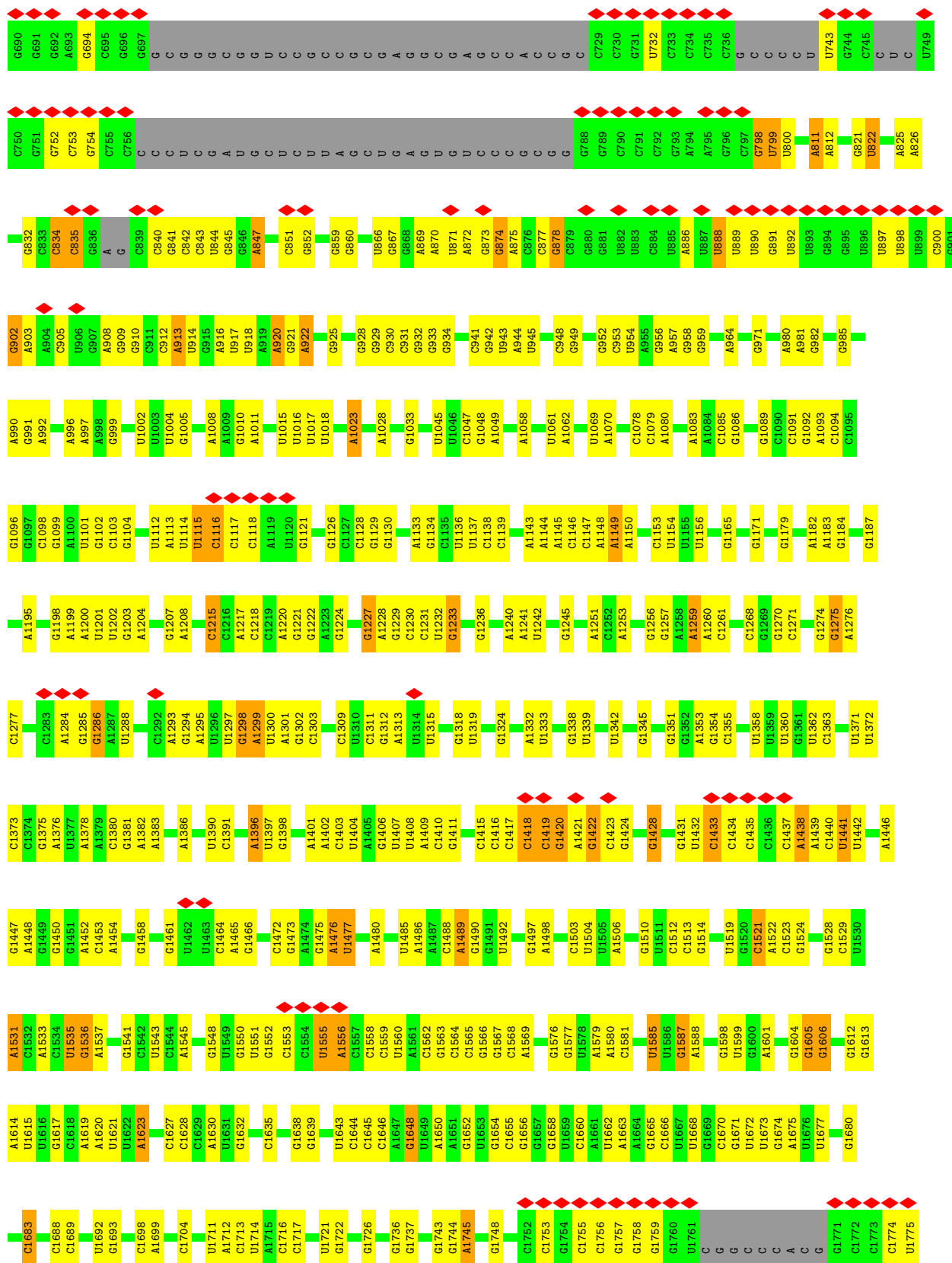
Chain YA: 



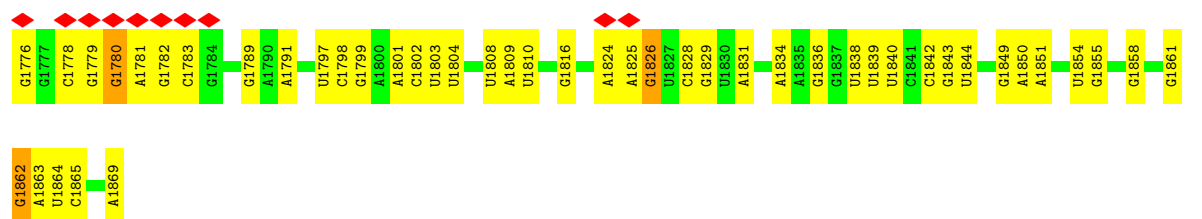
• Molecule 51: 18S rRNA

Chain ZA: 

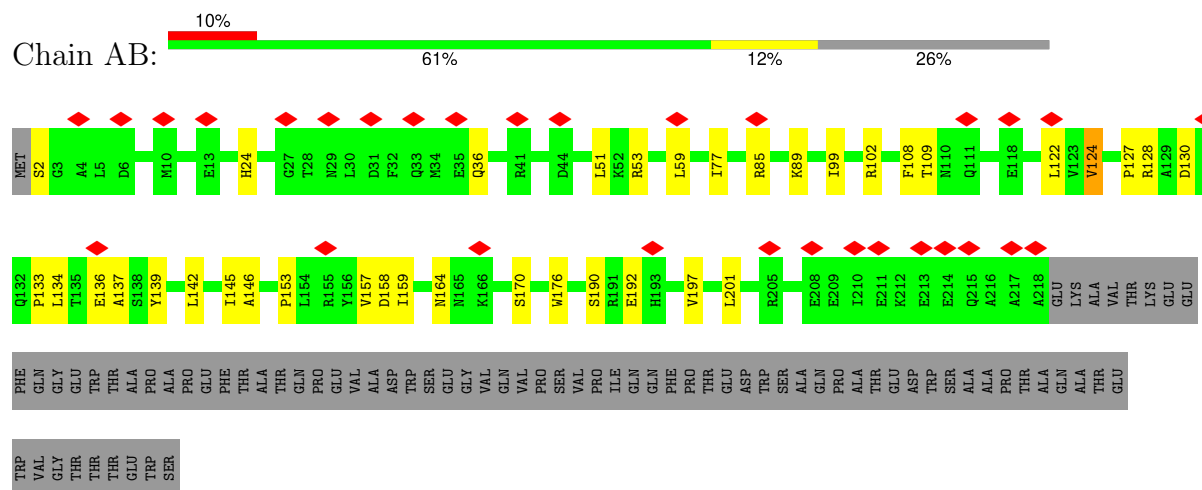




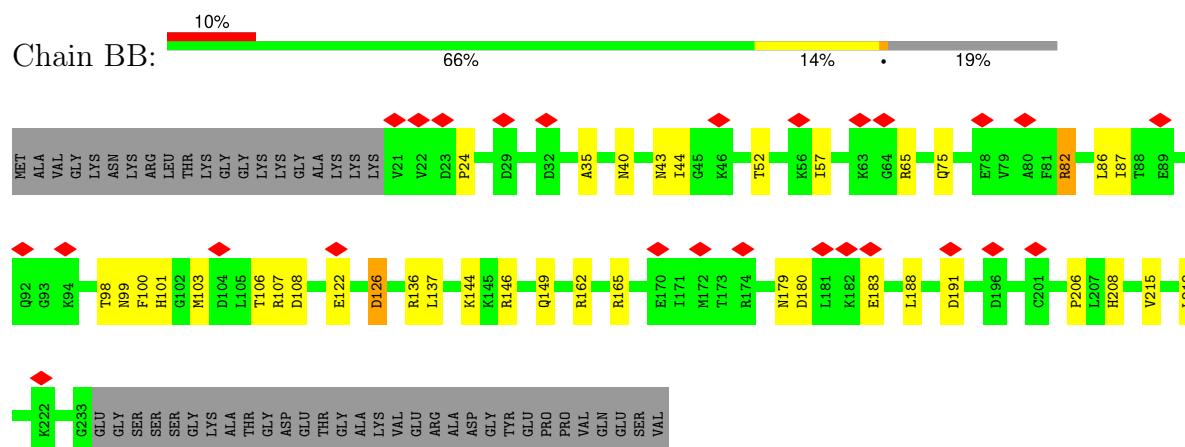




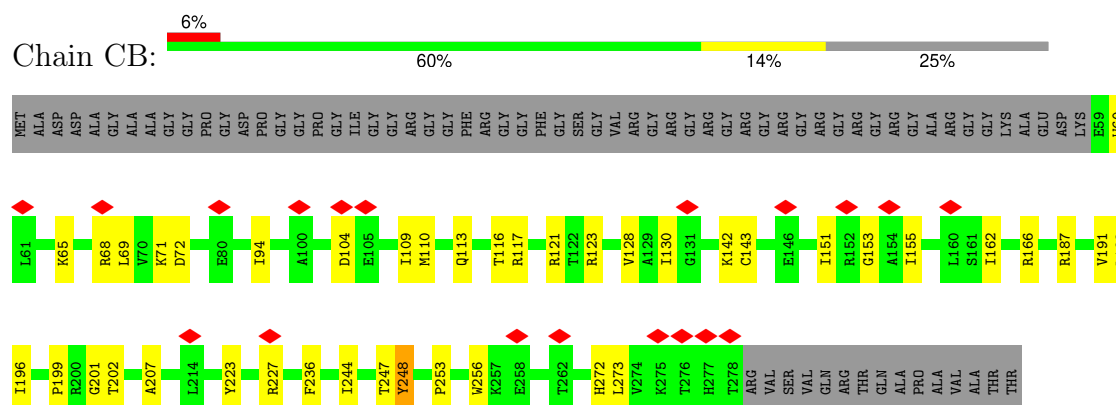
• Molecule 52: RPSA



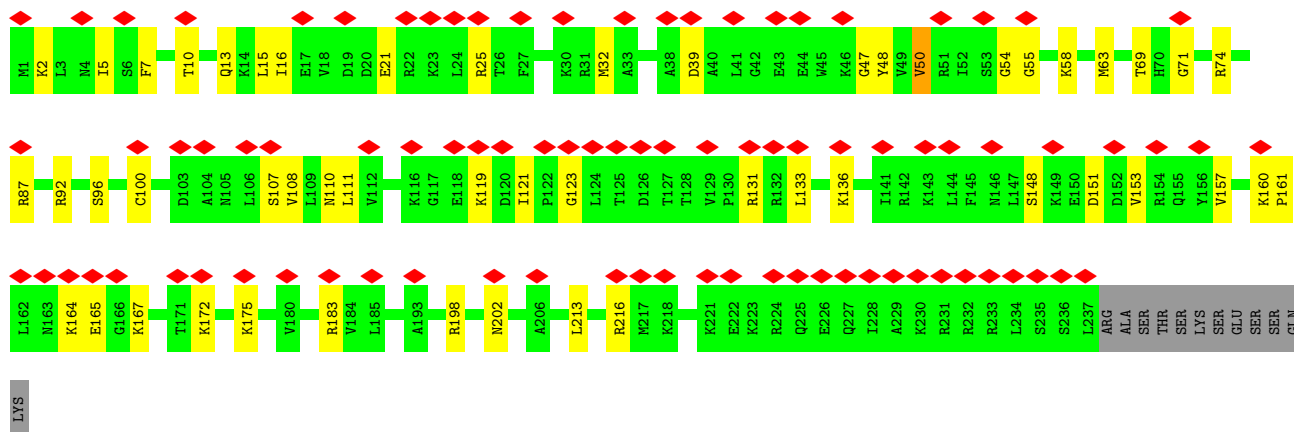
• Molecule 53: S3A



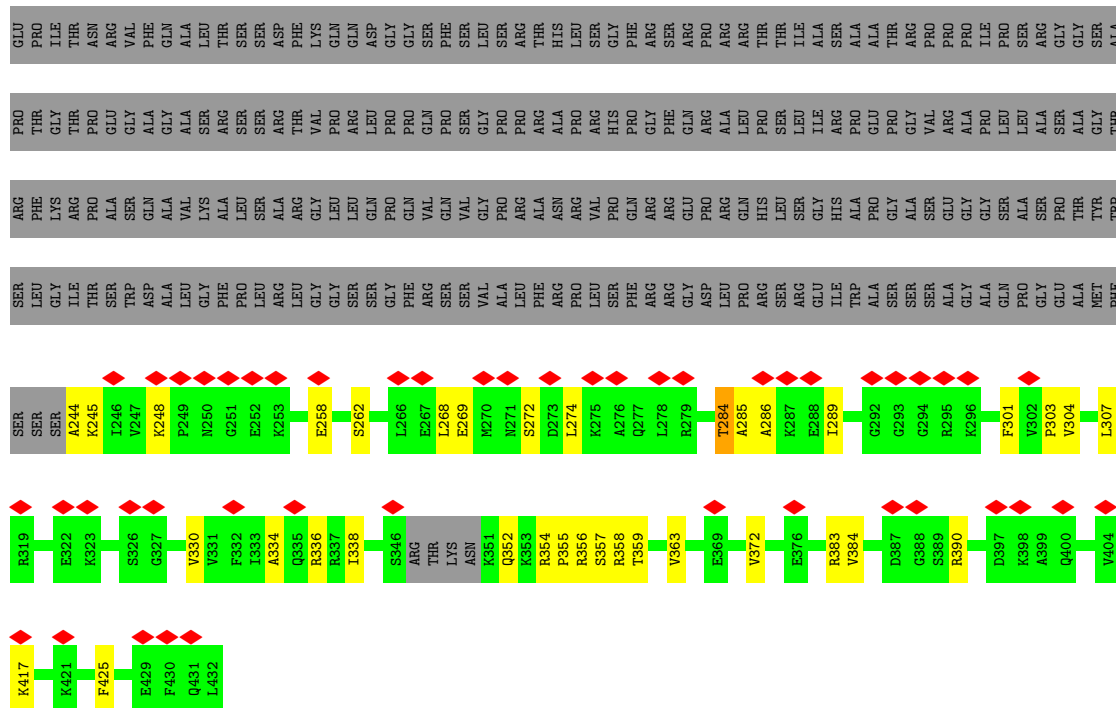
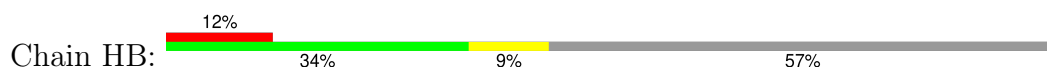
• Molecule 54: eS1



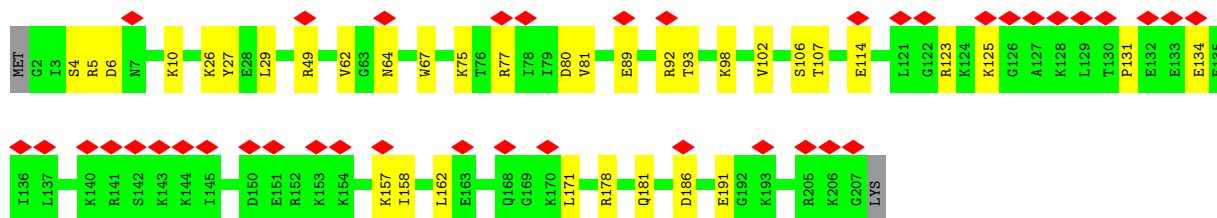
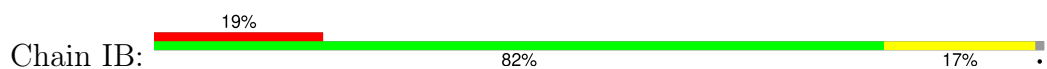




• Molecule 59: eS7

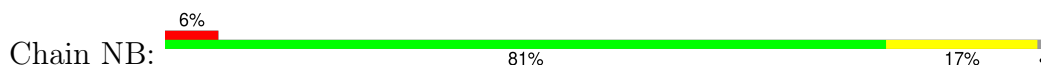


• Molecule 60: S8

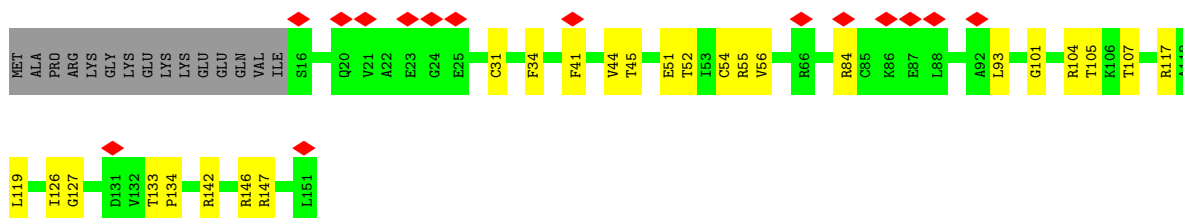
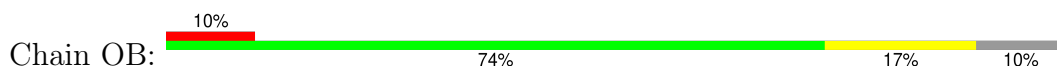


• Molecule 61: S9

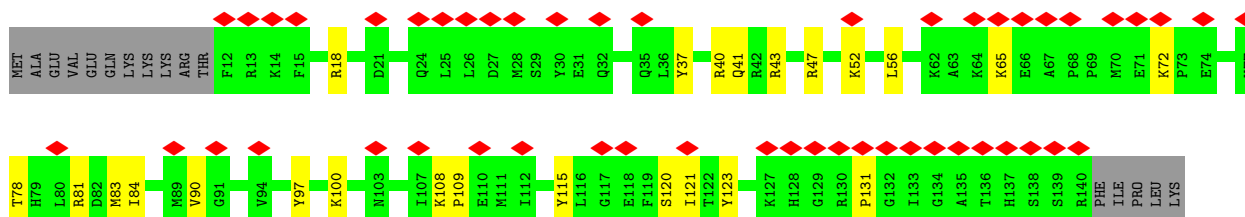
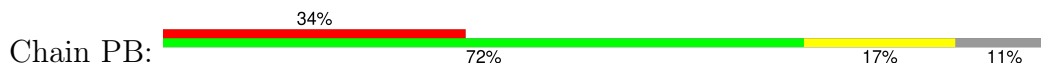




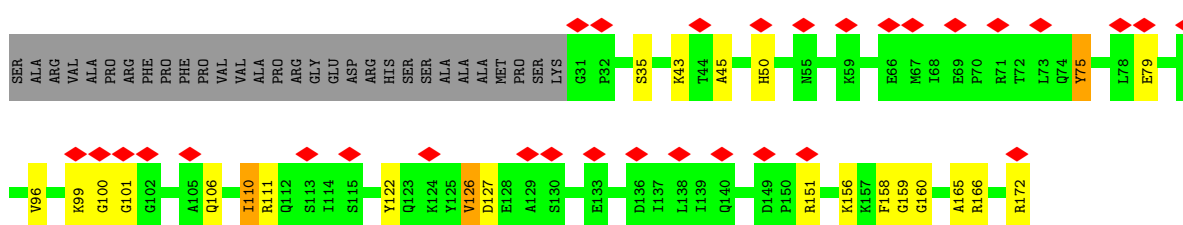
• Molecule 66: S14



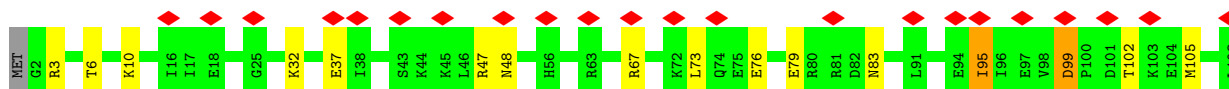
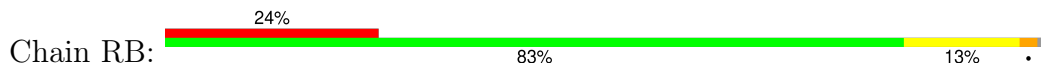
• Molecule 67: S15

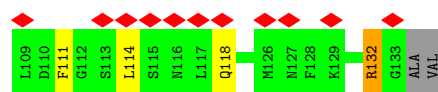


• Molecule 68: uS9



• Molecule 69: eS17

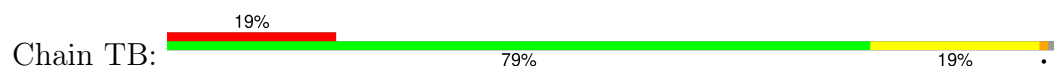




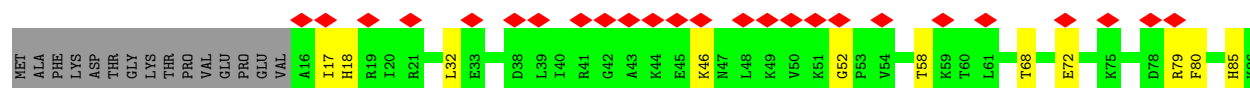
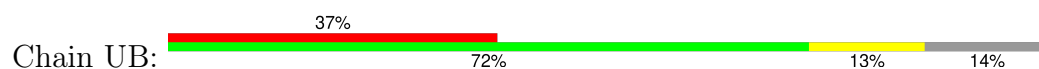
• Molecule 70: S18



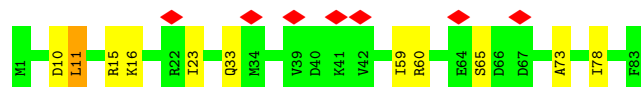
• Molecule 71: S19



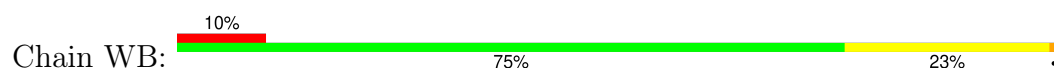
• Molecule 72: uS10

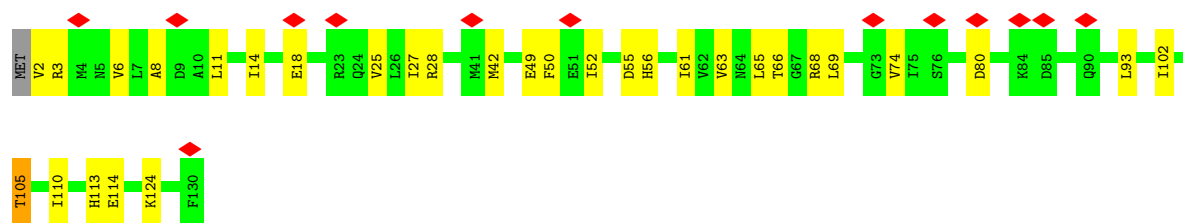


• Molecule 73: S21

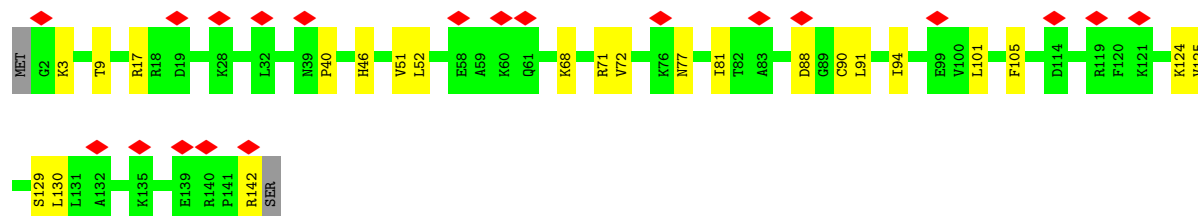
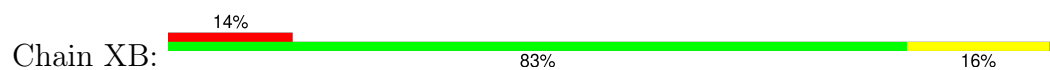


• Molecule 74: S15A

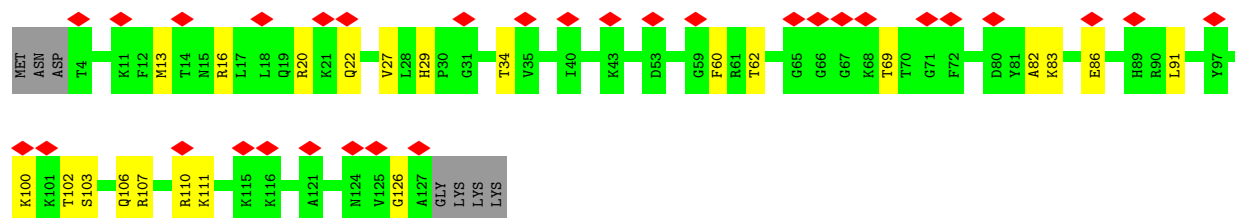
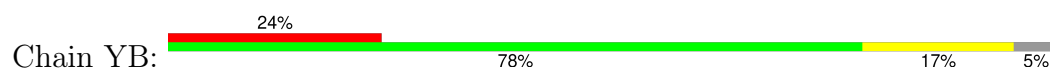




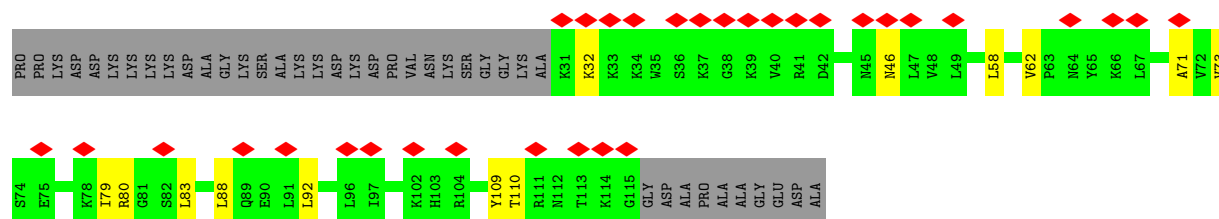
• Molecule 75: S23



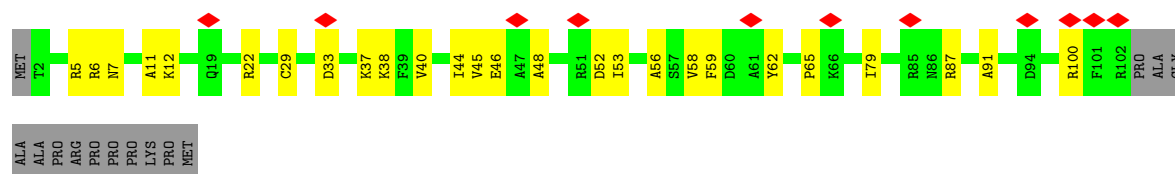
• Molecule 76: S24



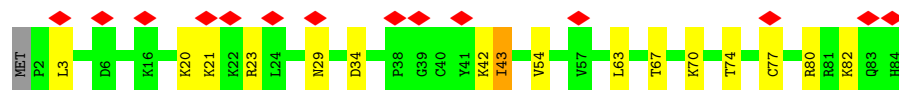
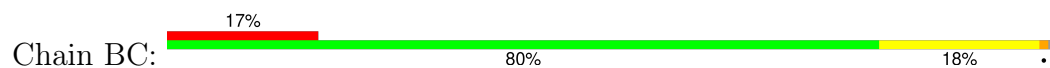
• Molecule 77: eS25



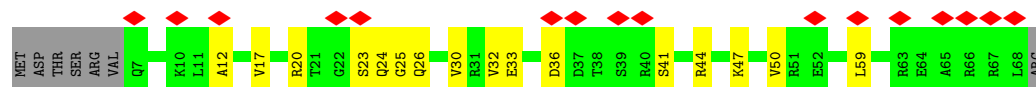
• Molecule 78: S26



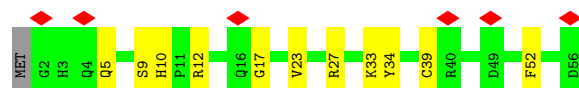
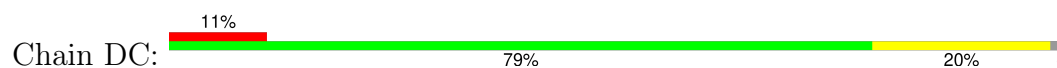
- Molecule 79: S27



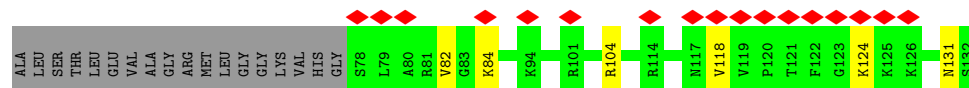
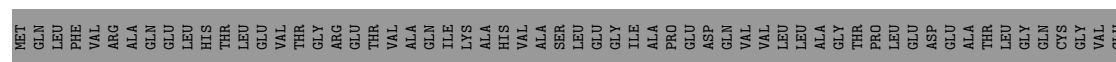
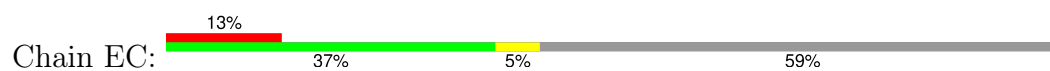
- Molecule 80: S28



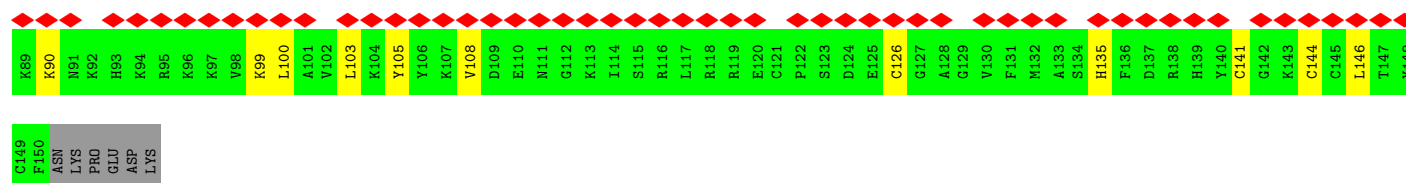
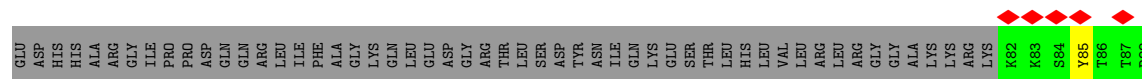
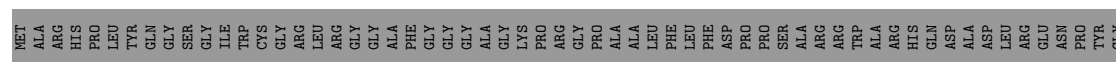
- Molecule 81: uS14



- Molecule 82: S30

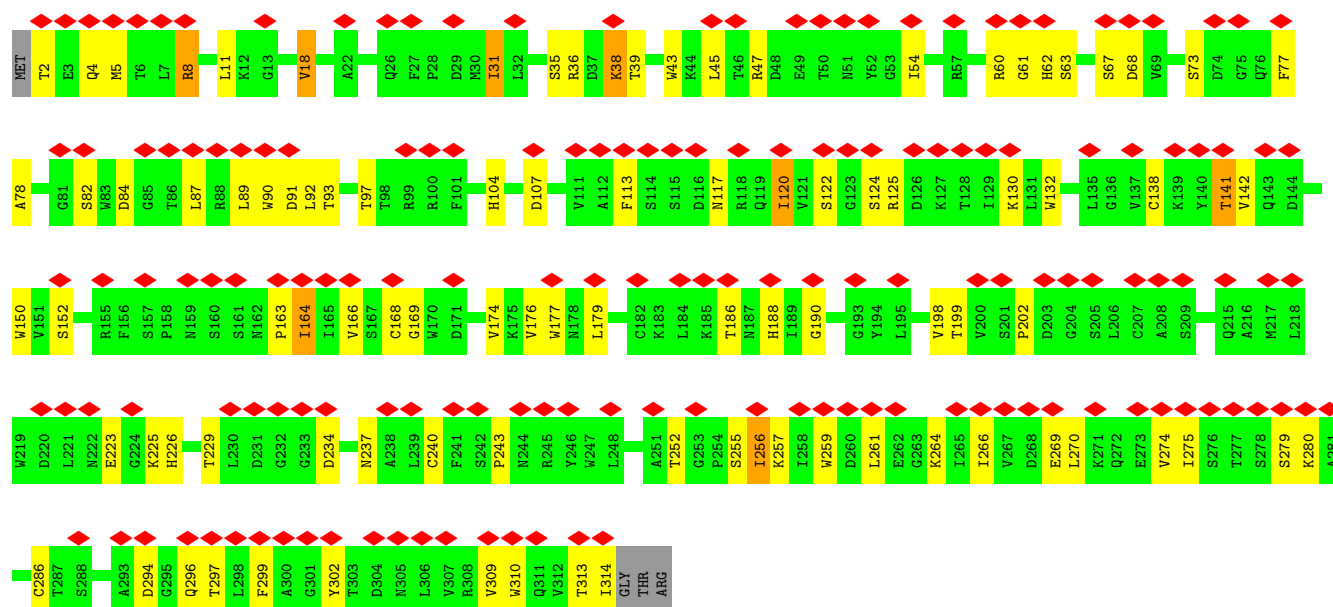


- Molecule 83: S27A

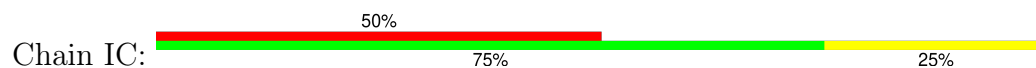


- Molecule 84: RACK1

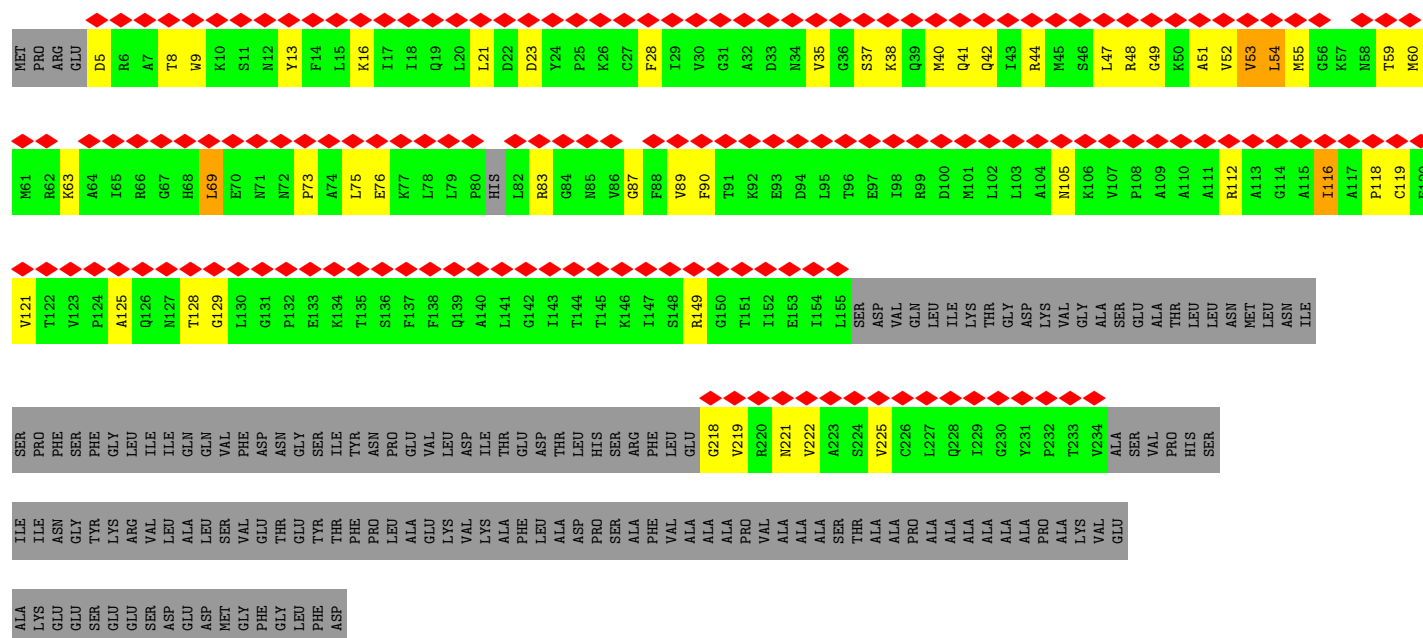
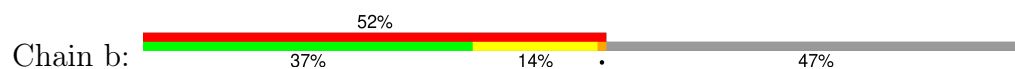




• Molecule 85: peptide



• Molecule 86: RPLP0

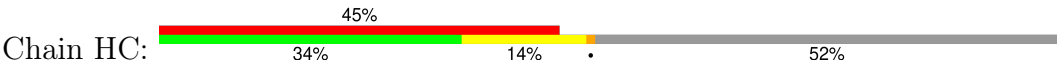


● Molecule 87: RPLP peptide



|      |      |      |      |      |      |      |      |      |      |      |      |      |      |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| S241 | E242 | E243 | S244 | D245 | E246 | D247 | W248 | G249 | F250 | G251 | L252 | F253 | D254 |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|

● Molecule 88: eukaryotic elongation factor 1A



|     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| MET | GLY | LYS | GLU | LYS | THR | HIS | ILE | ASN | VAL | VAL | ILE | GLY | HIS | VAL | ASP | SER | GLY | LYS | SER | THR | THR | THR | GLY | HIS | LEU | LEU | ILE | TYR | ILE | LYS | CYS | GLY | GLY | ILE | ASP | LYS | ARG | THR | THR | ILE | LYS | GLU | LYS | ASP | LYS | GLY | ALA | ALA | ALA | GLN | GLU | MET | GLY | ASP | LYS | VAL | THR | ALA | ALA | TRP | GLY | VAL | LEU |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

|     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| ASP | LYS | LEU | LYS | ALA | GLU | ARG | GLU | ARG | GLY | ILE | THR | ILE | ASP | GLY | HIS | SER | LEU | TRP | LYS | PHE | LYS | GLU | THR | THR | VAL | GLN | LEU | THR | ILE | ILE | ILE | ASP | ALA | PRO | GLY | LYS | HIS | ASP | ARG | ASP | THR | PHE | ILE | LYS | PRO | ASN | MET | LYS | ILE | THR | GLY | THR | GLY | THR | ALA | GLN | ASP | GLY | ASP | LYS | VAL | THR | ALA | ALA | TRP | GLY | VAL | LEU |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

|     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| GLY | GLU | PHE | GLU | ALA | GLY | ILE | SER | ASN | LYS | GLY | GLN | THR | ARG | GLY | GLU | HIS | ALA | LEU | LEU | ALA | ALA | LYS | VAL | TYR | THR | THR | LEU | LEU | ILE | ILE | VAL | GLY | VAL | ASN | GLY | ASP | LYS | MET | LYS | ASP | THR | THR | GLY | PRO | PRO | TYR | SER | GLN | LYS | ARG | THR | TYR | GLU | GLY | ILE | VAL | LYS | GLU | VAL | THR | THR | ILE | TYR | ALA | ALA | TRP | GLY | VAL | LEU |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

|     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |      |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|
| ILE | GLY | TYR | ASN | PRO | THR | THR | VAL | PHE | VAL | PRO | PRO | ILE | SER | GLY | TRP | GLY | ASP | ASN | MET | GLU | GLU | PRO | SER | ALA | ALA | ASN | MET | PRO | PRO | TRP | PHE | LYS | GLY | TRP | VAL | THR | THR | THR | ARG | ARG | LYS | ASP | GLY | ALA | SER | GLY | THR | THR | THR | LEU | GLY | GLU | ALA | ASP | CYS | ILE | LEU | PRO | PRO | THR | R240 |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|

|      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| P241 | T242 | D243 | K244 | P245 | L246 | R247 | L248 | P249 | L249 | Q251 | D252 | V253 | V254 | K255 | T256 | G257 | G258 | T259 | G260 | T261 | V262 | P263 | V264 | G265 | R266 | V267 | E268 | T269 | G270 | V271 | L272 | K273 | P274 | G275 | H276 | V277 | V278 | T279 | F280 | A281 | P282 | V283 | N284 | V285 | T286 | T287 | E288 | V289 | K290 | S291 | V292 | E293 | N294 | H295 | H296 | E297 | A298 | L299 | S300 |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|

|      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| E301 | A302 | L303 | P304 | G305 | D306 | N307 | V308 | G309 | F310 | N311 | V312 | K313 | N314 | V315 | S316 | V317 | K318 | D319 | V320 | R321 | R322 | G323 | N324 | V325 | A326 | G327 | D328 | S329 | K330 | N331 | D332 | F333 | P334 | M335 | E336 | A337 | A338 | G339 | F340 | T341 | A342 | G343 | V344 | I345 | I346 | L347 | N348 | H349 | P350 | G351 | Q352 | I353 | S354 | A355 | G356 | Y357 | A358 | F359 | V360 |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|

|      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| L361 | D362 | C363 | H364 | T365 | A366 | H367 | T368 | A369 | C370 | K371 | F372 | A373 | E374 | L375 | K376 | E377 | K378 | I379 | D380 | R381 | R382 | S383 | G384 | K385 | K386 | L387 | E388 | D389 | G390 | P391 | K392 | F393 | L394 | K395 | S396 | G397 | D398 | A399 | A400 | I401 | V402 | D403 | M404 | V405 | P406 | G407 | K408 | P409 | M410 | C411 | V412 | E413 | S414 | F415 | S416 | D417 | Y418 | P419 | P420 |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|

|      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| L421 | G422 | R423 | F424 | A425 | V426 | R427 | D428 | M429 | R430 | Q431 | T432 | V433 | A434 | V435 | G436 | V437 | T438 | K439 | A440 | V441 | D442 | K443 | K444 | A445 | A446 | G447 | A448 | G449 | K450 | V451 | T452 | K453 | S454 | A455 | Q456 | K457 | A458 | Q459 | K460 | A461 | K462 |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|

## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 5498                                    | 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 ( $e^-/\text{\AA}^2$ ) | 75                                      | Depositor |
| Minimum defocus (nm)                 | 500                                     | Depositor |
| Maximum defocus (nm)                 | 2500                                    | Depositor |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K3 (6k x 4k)                      | Depositor |
| Maximum map value                    | 33.748                                  | Depositor |
| Minimum map value                    | -22.021                                 | Depositor |
| Average map value                    | 0.004                                   | Depositor |
| Map value standard deviation         | 1.548                                   | Depositor |
| Recommended contour level            | 6                                       | Depositor |
| Map size ( $\text{\AA}$ )            | 686.87994, 686.87994, 686.87994         | wwPDB     |
| Map dimensions                       | 648, 648, 648                           | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 1.06, 1.06, 1.06                        | Depositor |

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, K, 5GP, ANM, SPD, MG

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

| Mol | Chain | Bond lengths |             | Bond angles |             |
|-----|-------|--------------|-------------|-------------|-------------|
|     |       | RMSZ         | $\# Z  > 5$ | RMSZ        | $\# Z  > 5$ |
| 1   | A     | 0.12         | 0/1952      | 0.28        | 0/2617      |
| 2   | B     | 0.12         | 0/3264      | 0.28        | 0/4371      |
| 3   | C     | 0.11         | 0/2937      | 0.25        | 0/3946      |
| 4   | D     | 0.10         | 0/2441      | 0.24        | 0/3269      |
| 5   | E     | 0.10         | 0/1859      | 0.26        | 0/2491      |
| 6   | F     | 0.11         | 0/1933      | 0.27        | 0/2577      |
| 7   | G     | 0.11         | 0/1881      | 0.26        | 0/2532      |
| 8   | H     | 0.11         | 0/1535      | 0.28        | 0/2063      |
| 9   | I     | 0.11         | 0/1702      | 0.24        | 0/2272      |
| 10  | J     | 0.10         | 0/1395      | 0.28        | 0/1863      |
| 11  | K     | 0.10         | 0/1733      | 0.25        | 0/2316      |
| 12  | L     | 0.11         | 0/1158      | 0.26        | 0/1547      |
| 13  | M     | 0.12         | 0/1746      | 0.27        | 0/2338      |
| 14  | N     | 0.12         | 0/1662      | 0.28        | 0/2222      |
| 15  | O     | 0.11         | 0/1292      | 0.29        | 0/1733      |
| 16  | P     | 0.11         | 0/1539      | 0.28        | 0/2054      |
| 17  | Q     | 0.10         | 0/1524      | 0.25        | 0/2013      |
| 18  | R     | 0.11         | 0/1501      | 0.28        | 0/2012      |
| 19  | S     | 0.10         | 0/1326      | 0.24        | 0/1770      |
| 20  | T     | 0.11         | 0/840       | 0.31        | 0/1127      |
| 21  | U     | 0.12         | 0/1018      | 0.27        | 0/1364      |
| 22  | V     | 0.11         | 0/900       | 0.27        | 0/1194      |
| 23  | W     | 0.10         | 0/984       | 0.25        | 0/1323      |
| 24  | X     | 0.10         | 0/1132      | 0.23        | 0/1504      |
| 25  | Y     | 0.11         | 0/1130      | 0.24        | 0/1507      |
| 26  | Z     | 0.11         | 0/1191      | 0.26        | 0/1590      |
| 27  | AA    | 0.08         | 0/886       | 0.20        | 0/1171      |
| 28  | BA    | 0.10         | 0/779       | 0.23        | 0/1044      |
| 29  | CA    | 0.11         | 0/908       | 0.27        | 0/1223      |
| 30  | DA    | 0.11         | 0/1082      | 0.24        | 0/1443      |
| 31  | EA    | 0.12         | 0/895       | 0.27        | 0/1198      |
| 32  | FA    | 0.11         | 0/916       | 0.28        | 0/1220      |

| Mol | Chain | Bond lengths |         | Bond angles |          |
|-----|-------|--------------|---------|-------------|----------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5  |
| 33  | GA    | 0.09         | 0/1016  | 0.24        | 0/1341   |
| 34  | HA    | 0.09         | 0/841   | 0.23        | 0/1112   |
| 35  | IA    | 0.11         | 0/731   | 0.26        | 0/966    |
| 36  | JA    | 0.09         | 0/575   | 0.26        | 0/761    |
| 37  | KA    | 0.11         | 0/459   | 0.27        | 0/608    |
| 38  | LA    | 0.10         | 0/435   | 0.26        | 0/575    |
| 39  | MA    | 0.09         | 0/240   | 0.19        | 0/305    |
| 40  | NA    | 0.10         | 0/864   | 0.23        | 0/1140   |
| 41  | OA    | 0.12         | 0/718   | 0.32        | 0/953    |
| 42  | PA    | 0.12         | 0/1010  | 0.30        | 0/1354   |
| 43  | RA    | 0.12         | 0/1174  | 0.32        | 0/1582   |
| 44  | SA    | 0.10         | 0/1815  | 0.23        | 0/2828   |
| 45  | TA    | 0.09         | 0/1804  | 0.23        | 0/2810   |
| 46  | UA    | 0.13         | 0/1783  | 0.32        | 0/2776   |
| 47  | VA    | 0.08         | 0/279   | 0.21        | 0/431    |
| 48  | WA    | 0.12         | 0/85839 | 0.25        | 0/133881 |
| 49  | XA    | 0.11         | 0/2836  | 0.20        | 0/4421   |
| 50  | YA    | 0.11         | 0/3701  | 0.24        | 0/5766   |
| 51  | ZA    | 0.11         | 0/40949 | 0.25        | 0/63819  |
| 52  | AB    | 0.11         | 0/1747  | 0.26        | 0/2374   |
| 53  | BB    | 0.10         | 0/1756  | 0.26        | 0/2350   |
| 54  | CB    | 0.12         | 0/1744  | 0.29        | 0/2358   |
| 55  | DB    | 0.10         | 0/1796  | 0.25        | 0/2417   |
| 56  | EB    | 0.11         | 0/2118  | 0.30        | 0/2849   |
| 57  | FB    | 0.11         | 0/1492  | 0.29        | 0/2005   |
| 58  | GB    | 0.10         | 0/1946  | 0.25        | 0/2590   |
| 59  | HB    | 0.10         | 0/1511  | 0.27        | 0/2022   |
| 60  | IB    | 0.11         | 0/1715  | 0.27        | 0/2287   |
| 61  | JB    | 0.10         | 0/1550  | 0.27        | 0/2069   |
| 62  | KB    | 0.10         | 0/834   | 0.28        | 0/1125   |
| 63  | LB    | 0.10         | 0/1200  | 0.25        | 0/1604   |
| 64  | MB    | 0.10         | 0/918   | 0.29        | 0/1233   |
| 65  | NB    | 0.10         | 0/1226  | 0.23        | 0/1649   |
| 66  | OB    | 0.11         | 0/1029  | 0.28        | 0/1380   |
| 67  | PB    | 0.13         | 0/1079  | 0.29        | 0/1441   |
| 68  | QB    | 0.12         | 0/1146  | 0.30        | 0/1534   |
| 69  | RB    | 0.10         | 0/1082  | 0.26        | 0/1452   |
| 70  | SB    | 0.10         | 0/1208  | 0.28        | 0/1618   |
| 71  | TB    | 0.10         | 0/1123  | 0.25        | 0/1504   |
| 72  | UB    | 0.10         | 0/818   | 0.28        | 0/1099   |
| 73  | VB    | 0.10         | 0/643   | 0.27        | 0/860    |
| 74  | WB    | 0.11         | 0/1051  | 0.31        | 0/1406   |
| 75  | XB    | 0.10         | 0/1116  | 0.26        | 0/1490   |

| Mol | Chain | Bond lengths |          | Bond angles |          |
|-----|-------|--------------|----------|-------------|----------|
|     |       | RMSZ         | # Z  >5  | RMSZ        | # Z  >5  |
| 76  | YB    | 0.10         | 0/1028   | 0.28        | 0/1366   |
| 77  | ZB    | 0.10         | 0/691    | 0.25        | 0/922    |
| 78  | AC    | 0.11         | 0/828    | 0.27        | 0/1109   |
| 79  | BC    | 0.08         | 0/665    | 0.23        | 0/891    |
| 80  | CC    | 0.09         | 0/490    | 0.25        | 0/656    |
| 81  | DC    | 0.09         | 0/470    | 0.24        | 0/623    |
| 82  | EC    | 0.08         | 0/447    | 0.23        | 0/587    |
| 83  | FC    | 0.10         | 0/576    | 0.27        | 0/764    |
| 84  | GC    | 0.11         | 0/2493   | 0.31        | 0/3394   |
| 85  | IC    | 0.05         | 0/19     | 0.15        | 0/25     |
| 86  | b     | 0.14         | 0/1296   | 0.32        | 0/1745   |
| 87  | c     | 0.12         | 0/111    | 0.30        | 0/145    |
| 88  | HC    | 0.11         | 0/1694   | 0.29        | 0/2287   |
| All | All   | 0.11         | 0/236766 | 0.25        | 0/347573 |

There are no bond length outliers.

There are no bond angle outliers.

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   | A     | 1914  | 0        | 2013     | 40      | 0            |
| 2   | B     | 3196  | 0        | 3339     | 53      | 0            |
| 3   | C     | 2883  | 0        | 3053     | 32      | 0            |
| 4   | D     | 2395  | 0        | 2427     | 29      | 0            |
| 5   | E     | 1823  | 0        | 1995     | 29      | 0            |
| 6   | F     | 1897  | 0        | 2021     | 33      | 0            |
| 7   | G     | 1850  | 0        | 1991     | 25      | 0            |
| 8   | H     | 1516  | 0        | 1597     | 13      | 0            |
| 9   | I     | 1664  | 0        | 1712     | 22      | 0            |
| 10  | J     | 1372  | 0        | 1412     | 23      | 0            |
| 11  | K     | 1702  | 0        | 1820     | 25      | 0            |
| 12  | L     | 1137  | 0        | 1211     | 21      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 13  | M     | 1701  | 0        | 1749     | 37      | 0            |
| 14  | N     | 1630  | 0        | 1778     | 30      | 0            |
| 15  | O     | 1266  | 0        | 1302     | 15      | 0            |
| 16  | P     | 1515  | 0        | 1634     | 35      | 0            |
| 17  | Q     | 1508  | 0        | 1664     | 20      | 0            |
| 18  | R     | 1462  | 0        | 1508     | 25      | 0            |
| 19  | S     | 1298  | 0        | 1366     | 24      | 0            |
| 20  | T     | 826   | 0        | 852      | 14      | 0            |
| 21  | U     | 1004  | 0        | 1063     | 15      | 0            |
| 22  | V     | 887   | 0        | 935      | 11      | 0            |
| 23  | W     | 967   | 0        | 1040     | 11      | 0            |
| 24  | X     | 1115  | 0        | 1205     | 16      | 0            |
| 25  | Y     | 1107  | 0        | 1182     | 24      | 0            |
| 26  | Z     | 1162  | 0        | 1209     | 24      | 0            |
| 27  | AA    | 873   | 0        | 949      | 10      | 0            |
| 28  | BA    | 769   | 0        | 803      | 11      | 0            |
| 29  | CA    | 893   | 0        | 932      | 15      | 0            |
| 30  | DA    | 1064  | 0        | 1160     | 20      | 0            |
| 31  | EA    | 876   | 0        | 912      | 10      | 0            |
| 32  | FA    | 906   | 0        | 998      | 5       | 0            |
| 33  | GA    | 1008  | 0        | 1142     | 22      | 0            |
| 34  | HA    | 830   | 0        | 916      | 6       | 0            |
| 35  | IA    | 716   | 0        | 750      | 16      | 0            |
| 36  | JA    | 569   | 0        | 637      | 9       | 0            |
| 37  | KA    | 447   | 0        | 480      | 14      | 0            |
| 38  | LA    | 429   | 0        | 465      | 7       | 0            |
| 39  | MA    | 239   | 0        | 289      | 3       | 0            |
| 40  | NA    | 851   | 0        | 920      | 15      | 0            |
| 41  | OA    | 708   | 0        | 757      | 7       | 0            |
| 42  | PA    | 994   | 0        | 1051     | 18      | 0            |
| 43  | RA    | 1160  | 0        | 1218     | 18      | 0            |
| 44  | SA    | 1622  | 0        | 825      | 15      | 0            |
| 45  | TA    | 1615  | 0        | 820      | 14      | 0            |
| 46  | UA    | 1596  | 0        | 810      | 19      | 0            |
| 47  | VA    | 251   | 0        | 128      | 2       | 0            |
| 48  | WA    | 76735 | 0        | 38762    | 941     | 0            |
| 49  | XA    | 2538  | 0        | 1286     | 28      | 0            |
| 50  | YA    | 3314  | 0        | 1683     | 40      | 0            |
| 51  | ZA    | 36623 | 0        | 18504    | 475     | 0            |
| 52  | AB    | 1710  | 0        | 1711     | 23      | 0            |
| 53  | BB    | 1729  | 0        | 1803     | 23      | 0            |
| 54  | CB    | 1707  | 0        | 1793     | 28      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 55  | DB    | 1768  | 0        | 1863     | 21      | 0            |
| 56  | EB    | 2076  | 0        | 2177     | 36      | 0            |
| 57  | FB    | 1471  | 0        | 1522     | 24      | 0            |
| 58  | GB    | 1923  | 0        | 2089     | 38      | 0            |
| 59  | HB    | 1489  | 0        | 1582     | 25      | 0            |
| 60  | IB    | 1686  | 0        | 1772     | 23      | 0            |
| 61  | JB    | 1525  | 0        | 1640     | 27      | 0            |
| 62  | KB    | 810   | 0        | 836      | 21      | 0            |
| 63  | LB    | 1180  | 0        | 1254     | 14      | 0            |
| 64  | MB    | 908   | 0        | 939      | 19      | 0            |
| 65  | NB    | 1202  | 0        | 1289     | 18      | 0            |
| 66  | OB    | 1016  | 0        | 1039     | 20      | 0            |
| 67  | PB    | 1058  | 0        | 1104     | 17      | 0            |
| 68  | QB    | 1128  | 0        | 1195     | 17      | 0            |
| 69  | RB    | 1068  | 0        | 1121     | 15      | 0            |
| 70  | SB    | 1190  | 0        | 1249     | 30      | 0            |
| 71  | TB    | 1104  | 0        | 1140     | 20      | 0            |
| 72  | UB    | 808   | 0        | 878      | 13      | 0            |
| 73  | VB    | 636   | 0        | 637      | 8       | 0            |
| 74  | WB    | 1034  | 0        | 1080     | 22      | 0            |
| 75  | XB    | 1098  | 0        | 1167     | 15      | 0            |
| 76  | YB    | 1011  | 0        | 1083     | 19      | 0            |
| 77  | ZB    | 683   | 0        | 761      | 9       | 0            |
| 78  | AC    | 814   | 0        | 864      | 19      | 0            |
| 79  | BC    | 651   | 0        | 672      | 9       | 0            |
| 80  | CC    | 488   | 0        | 514      | 12      | 0            |
| 81  | DC    | 459   | 0        | 449      | 8       | 0            |
| 82  | EC    | 443   | 0        | 492      | 7       | 0            |
| 83  | FC    | 564   | 0        | 577      | 7       | 0            |
| 84  | GC    | 2436  | 0        | 2393     | 49      | 0            |
| 85  | IC    | 20    | 0        | 10       | 1       | 0            |
| 86  | b     | 1279  | 0        | 1343     | 34      | 0            |
| 87  | c     | 110   | 0        | 83       | 4       | 0            |
| 88  | HC    | 1664  | 0        | 1721     | 31      | 0            |
| 89  | A     | 1     | 0        | 0        | 0       | 0            |
| 89  | AC    | 1     | 0        | 0        | 0       | 0            |
| 89  | FA    | 1     | 0        | 0        | 0       | 0            |
| 89  | HC    | 1     | 0        | 0        | 0       | 0            |
| 89  | I     | 1     | 0        | 0        | 0       | 0            |
| 89  | IA    | 1     | 0        | 0        | 0       | 0            |
| 89  | O     | 1     | 0        | 0        | 0       | 0            |
| 89  | P     | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 89  | U     | 1      | 0        | 0        | 0       | 0            |
| 89  | VA    | 1      | 0        | 0        | 0       | 0            |
| 89  | WA    | 142    | 0        | 0        | 0       | 0            |
| 89  | XA    | 4      | 0        | 0        | 0       | 0            |
| 89  | YA    | 2      | 0        | 0        | 0       | 0            |
| 89  | Z     | 1      | 0        | 0        | 0       | 0            |
| 89  | ZA    | 45     | 0        | 0        | 0       | 0            |
| 90  | AC    | 1      | 0        | 0        | 0       | 0            |
| 90  | DC    | 1      | 0        | 0        | 0       | 0            |
| 90  | FA    | 1      | 0        | 0        | 0       | 0            |
| 90  | FC    | 1      | 0        | 0        | 0       | 0            |
| 90  | IA    | 1      | 0        | 0        | 0       | 0            |
| 90  | LA    | 1      | 0        | 0        | 0       | 0            |
| 90  | NA    | 1      | 0        | 0        | 0       | 0            |
| 90  | OA    | 1      | 0        | 0        | 0       | 0            |
| 91  | UA    | 24     | 0        | 11       | 0       | 0            |
| 92  | WA    | 19     | 0        | 18       | 1       | 0            |
| 93  | WA    | 20     | 0        | 38       | 1       | 0            |
| 93  | ZA    | 10     | 0        | 19       | 0       | 0            |
| 94  | WA    | 1      | 0        | 0        | 0       | 0            |
| 95  | HC    | 6      | 0        | 4        | 0       | 0            |
| All | All   | 220661 | 0        | 164207   | 2523    | 0            |

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

All (2523) 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) |
|------------------|-------------------|--------------------------|-------------------|
| 48:WA:2847:A:H61 | 48:WA:3845:C:N4   | 1.54                     | 1.04              |
| 48:WA:2847:A:N6  | 48:WA:3845:C:H42  | 1.58                     | 1.00              |
| 51:ZA:197:U:H3   | 51:ZA:202:G:H1    | 1.04                     | 1.00              |
| 48:WA:1249:U:H3  | 48:WA:1268:G:H1   | 1.03                     | 0.96              |
| 51:ZA:1743:G:N2  | 51:ZA:1791:A:H62  | 1.64                     | 0.95              |
| 48:WA:1446:G:H1  | 48:WA:2113:U:H3   | 1.08                     | 0.92              |
| 51:ZA:1743:G:H21 | 51:ZA:1791:A:H62  | 0.95                     | 0.92              |
| 46:UA:8:U:H3     | 46:UA:14:A:H62    | 1.13                     | 0.91              |
| 44:SA:50:U:H3    | 44:SA:64:G:H1     | 0.97                     | 0.90              |
| 51:ZA:1472:C:H42 | 51:ZA:1476:A:H62  | 1.18                     | 0.90              |
| 55:DB:201:PRO:O  | 55:DB:205:TYR:HB2 | 1.72                     | 0.90              |
| 51:ZA:1656:G:H1  | 51:ZA:1668:U:H3   | 1.16                     | 0.89              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 51:ZA:1743:G:H21  | 51:ZA:1791:A:N6    | 1.69                     | 0.87              |
| 48:WA:2487:U:H3   | 48:WA:2495:G:H1    | 1.19                     | 0.85              |
| 51:ZA:1288:U:H3   | 51:ZA:1311:C:H42   | 1.24                     | 0.82              |
| 48:WA:2575:A:H62  | 48:WA:2763:U:H3    | 1.27                     | 0.81              |
| 48:WA:1761:G:H1   | 48:WA:1775:U:H3    | 1.25                     | 0.80              |
| 51:ZA:677:G:H21   | 51:ZA:1028:A:H62   | 1.31                     | 0.78              |
| 46:UA:8:U:H3      | 46:UA:14:A:N6      | 1.81                     | 0.77              |
| 56:EB:185:GLY:H   | 56:EB:189:LEU:HD13 | 1.48                     | 0.77              |
| 48:WA:4995:G:H1   | 48:WA:5060:A:H2    | 1.30                     | 0.77              |
| 86:b:55:MET:HG3   | 86:b:87:GLY:HA3    | 1.67                     | 0.76              |
| 74:WB:8:ALA:HA    | 74:WB:74:VAL:HG21  | 1.67                     | 0.76              |
| 48:WA:2847:A:H61  | 48:WA:3845:C:H42   | 0.81                     | 0.75              |
| 46:UA:10:G:H22    | 46:UA:25:C:H2'     | 1.51                     | 0.75              |
| 48:WA:2522:C:O2   | 48:WA:2642:G:N2    | 2.20                     | 0.74              |
| 35:IA:2:THR:N     | 48:WA:3644:A:HO2'  | 1.86                     | 0.73              |
| 51:ZA:1472:C:N4   | 51:ZA:1476:A:H62   | 1.86                     | 0.73              |
| 51:ZA:561:A:H5'   | 61:JB:171:GLY:HA3  | 1.71                     | 0.72              |
| 48:WA:1452:C:HO2' | 48:WA:2106:A:HO2'  | 1.36                     | 0.72              |
| 86:b:5:ASP:N      | 86:b:8:THR:HG1     | 1.87                     | 0.72              |
| 48:WA:1975:G:H2'  | 48:WA:1976:U:H2'   | 1.71                     | 0.72              |
| 51:ZA:1396:A:O2'  | 51:ZA:1398:G:N7    | 2.20                     | 0.72              |
| 48:WA:3699:U:H5'' | 48:WA:3700:G:H5'   | 1.72                     | 0.72              |
| 48:WA:4770:G:H2'  | 48:WA:4771:G:C8    | 2.25                     | 0.72              |
| 51:ZA:442:C:H42   | 51:ZA:449:A:H62    | 1.38                     | 0.72              |
| 48:WA:4874:G:H4'  | 48:WA:4875:G:H5'   | 1.72                     | 0.72              |
| 48:WA:4737:G:H1   | 48:WA:4967:U:H3    | 1.36                     | 0.71              |
| 58:GB:69:THR:HG22 | 58:GB:71:GLY:H     | 1.54                     | 0.71              |
| 5:E:48:ARG:HB2    | 5:E:64:MET:HE1     | 1.72                     | 0.71              |
| 3:C:78:ARG:HB3    | 3:C:88:GLY:HA2     | 1.72                     | 0.71              |
| 14:N:125:LYS:HG3  | 14:N:129:LEU:HD12  | 1.73                     | 0.70              |
| 48:WA:995:U:H3    | 48:WA:1071:G:H1    | 1.38                     | 0.70              |
| 10:J:75:ARG:NH1   | 49:XA:40:U:O2      | 2.25                     | 0.70              |
| 72:UB:80:PHE:HB3  | 81:DC:52:PHE:HB3   | 1.71                     | 0.70              |
| 69:RB:111:PHE:HB3 | 69:RB:114:LEU:HD11 | 1.73                     | 0.69              |
| 51:ZA:15:U:O2'    | 51:ZA:669:A:N6     | 2.25                     | 0.69              |
| 2:B:249:ARG:NH1   | 48:WA:2839:U:OP1   | 2.25                     | 0.69              |
| 11:K:56:ARG:O     | 11:K:116:ARG:NH1   | 2.25                     | 0.69              |
| 18:R:87:ARG:HH21  | 48:WA:2036:G:H5'   | 1.57                     | 0.69              |
| 5:E:115:MET:O     | 42:PA:87:ARG:NH1   | 2.26                     | 0.69              |
| 51:ZA:1298:G:HO2' | 51:ZA:1299:A:H8    | 1.40                     | 0.69              |
| 68:QB:96:VAL:HG11 | 68:QB:110:ILE:HG13 | 1.75                     | 0.69              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 51:ZA:959:G:OP1    | 66:OB:104:ARG:NH2 | 2.27                     | 0.68              |
| 51:ZA:1658:G:OP2   | 51:ZA:1660:C:N4   | 2.27                     | 0.68              |
| 71:TB:76:THR:HB    | 71:TB:94:ARG:HB3  | 1.75                     | 0.68              |
| 43:RA:121:LEU:HB2  | 86:b:49:GLY:HA2   | 1.76                     | 0.68              |
| 48:WA:3946:G:H1    | 48:WA:4071:U:H3   | 1.42                     | 0.68              |
| 51:ZA:1410:C:H2'   | 51:ZA:1411:G:H8   | 1.57                     | 0.68              |
| 18:R:34:ALA:HB1    | 18:R:39:VAL:HG23  | 1.76                     | 0.68              |
| 84:GC:256:ILE:HG23 | 84:GC:270:LEU:HB2 | 1.76                     | 0.68              |
| 84:GC:199:THR:HG21 | 84:GC:240:CYS:HA  | 1.77                     | 0.67              |
| 5:E:186:ARG:HH21   | 48:WA:4938:G:H2'  | 1.60                     | 0.67              |
| 48:WA:1526:A:H62   | 48:WA:1653:G:H1   | 1.42                     | 0.67              |
| 48:WA:2022:U:H2'   | 48:WA:2023:G:H8   | 1.59                     | 0.67              |
| 48:WA:3643:U:OP2   | 48:WA:3648:A:N6   | 2.27                     | 0.67              |
| 48:WA:4355:U:H5''  | 48:WA:4356:U:H5'  | 1.75                     | 0.67              |
| 48:WA:4995:G:O6    | 48:WA:5060:A:N1   | 2.27                     | 0.67              |
| 51:ZA:482:G:N1     | 51:ZA:485:A:OP2   | 2.27                     | 0.67              |
| 51:ZA:888:U:H2'    | 51:ZA:900:C:H42   | 1.58                     | 0.67              |
| 51:ZA:1674:G:OP1   | 57:FB:51:HIS:NE2  | 2.25                     | 0.67              |
| 45:TA:15:G:N2      | 45:TA:48:C:C2     | 2.62                     | 0.67              |
| 51:ZA:1091:C:HO2'  | 74:WB:2:VAL:N     | 1.93                     | 0.67              |
| 51:ZA:957:A:H3'    | 51:ZA:958:G:H21   | 1.60                     | 0.66              |
| 53:BB:107:ARG:NH1  | 66:OB:133:THR:O   | 2.27                     | 0.66              |
| 54:CB:123:ARG:NH1  | 54:CB:143:CYS:SG  | 2.68                     | 0.66              |
| 11:K:74:ARG:NH2    | 48:WA:109:G:OP2   | 2.29                     | 0.66              |
| 48:WA:1766:G:OP2   | 48:WA:1766:G:N2   | 2.28                     | 0.66              |
| 48:WA:3762:A:N6    | 51:ZA:1826:G:OP2  | 2.29                     | 0.66              |
| 19:S:70:HIS:NE2    | 48:WA:4329:C:OP1  | 2.29                     | 0.66              |
| 84:GC:31:ILE:HG23  | 84:GC:43:TRP:HB2  | 1.77                     | 0.66              |
| 6:F:227:VAL:HA     | 18:R:39:VAL:HG12  | 1.76                     | 0.66              |
| 48:WA:4696:G:OP1   | 48:WA:4696:G:N2   | 2.29                     | 0.66              |
| 26:Z:21:ARG:NH2    | 48:WA:1319:U:OP1  | 2.28                     | 0.66              |
| 51:ZA:1473:G:N2    | 51:ZA:1476:A:OP2  | 2.29                     | 0.66              |
| 38:LA:74:TYR:O     | 48:WA:4474:G:O2'  | 2.14                     | 0.65              |
| 51:ZA:377:G:H5'    | 60:IB:98:LYS:HB3  | 1.78                     | 0.65              |
| 3:C:340:ILE:HD13   | 5:E:53:VAL:HG21   | 1.78                     | 0.65              |
| 4:D:103:LEU:HD11   | 4:D:248:ARG:HE    | 1.61                     | 0.65              |
| 11:K:31:ARG:HD3    | 11:K:35:ARG:HH21  | 1.61                     | 0.65              |
| 48:WA:3694:A:H62   | 48:WA:3825:G:H21  | 1.43                     | 0.65              |
| 2:B:249:ARG:NH2    | 48:WA:3847:A:OP2  | 2.30                     | 0.65              |
| 51:ZA:1396:A:N7    | 51:ZA:1450:G:N2   | 2.45                     | 0.65              |
| 88:HC:380:ASP:HB3  | 88:HC:383:SER:HB2 | 1.79                     | 0.65              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 48:WA:1092:C:H2'   | 48:WA:1093:A:H8   | 1.61                     | 0.65              |
| 48:WA:4423:C:H42   | 48:WA:4477:G:H22  | 1.44                     | 0.65              |
| 25:Y:103:ASP:HB3   | 25:Y:106:LEU:HB2  | 1.79                     | 0.65              |
| 41:OA:4:ARG:NH2    | 48:WA:1557:G:O6   | 2.30                     | 0.65              |
| 48:WA:102:G:HO2'   | 48:WA:1383:U:HO2' | 1.44                     | 0.65              |
| 48:WA:1929:U:OP1   | 48:WA:1951:U:O2'  | 2.13                     | 0.65              |
| 51:ZA:114:G:N7     | 63:LB:69:ARG:NH2  | 2.45                     | 0.65              |
| 51:ZA:1403:C:N4    | 51:ZA:1433:C:OP1  | 2.30                     | 0.65              |
| 56:EB:122:LYS:NZ   | 56:EB:124:CYS:SG  | 2.68                     | 0.65              |
| 51:ZA:1298:G:H4'   | 67:PB:78:THR:HA   | 1.79                     | 0.64              |
| 37:KA:37:TYR:O     | 48:WA:362:A:N6    | 2.30                     | 0.64              |
| 66:OB:142:ARG:HB3  | 78:AC:22:ARG:HD3  | 1.80                     | 0.64              |
| 11:K:59:VAL:HB     | 48:WA:74:G:H5'    | 1.78                     | 0.64              |
| 48:WA:1334:C:H2'   | 48:WA:1335:A:H8   | 1.63                     | 0.64              |
| 8:H:85:THR:HG23    | 8:H:86:LEU:HG     | 1.78                     | 0.64              |
| 48:WA:4539:C:H2'   | 48:WA:4540:G:H8   | 1.63                     | 0.64              |
| 48:WA:4543:G:N2    | 48:WA:4546:A:OP2  | 2.28                     | 0.64              |
| 48:WA:1726:G:N2    | 48:WA:1878:U:OP1  | 2.31                     | 0.64              |
| 48:WA:1745:A:N1    | 48:WA:1791:C:O2'  | 2.29                     | 0.64              |
| 84:GC:39:THR:HG22  | 84:GC:60:ARG:HG2  | 1.80                     | 0.64              |
| 51:ZA:1130:G:N2    | 51:ZA:1130:G:OP2  | 2.31                     | 0.64              |
| 31:EA:100:ARG:NH1  | 48:WA:4755:U:OP1  | 2.31                     | 0.64              |
| 43:RA:17:CYS:O     | 43:RA:57:ARG:HA   | 1.98                     | 0.64              |
| 4:D:256:LYS:HD2    | 49:XA:117:G:H5'   | 1.80                     | 0.64              |
| 48:WA:970:G:N2     | 48:WA:2098:G:O2'  | 2.32                     | 0.64              |
| 48:WA:961:A:H1'    | 48:WA:2078:G:H5'' | 1.79                     | 0.63              |
| 74:WB:42:MET:HE2   | 74:WB:49:GLU:HA   | 1.80                     | 0.63              |
| 86:b:121:VAL:HG13  | 86:b:221:ASN:HD21 | 1.64                     | 0.63              |
| 19:S:43:LYS:NZ     | 48:WA:1735:G:OP1  | 2.31                     | 0.63              |
| 48:WA:1554:G:O2'   | 48:WA:1576:G:N2   | 2.32                     | 0.63              |
| 66:OB:105:THR:HG22 | 66:OB:107:THR:H   | 1.63                     | 0.63              |
| 24:X:15:ARG:NH1    | 48:WA:230:G:OP1   | 2.32                     | 0.63              |
| 35:IA:33:THR:HG22  | 35:IA:40:PRO:HG2  | 1.81                     | 0.63              |
| 48:WA:916:U:H4'    | 48:WA:917:A:H5'   | 1.81                     | 0.63              |
| 48:WA:1741:G:N3    | 48:WA:1744:A:N6   | 2.47                     | 0.63              |
| 56:EB:87:MET:HE2   | 56:EB:123:LEU:HB2 | 1.80                     | 0.63              |
| 51:ZA:649:U:H2'    | 51:ZA:650:A:H8    | 1.64                     | 0.63              |
| 51:ZA:851:C:H5''   | 51:ZA:852:G:H5'   | 1.80                     | 0.63              |
| 11:K:103:ARG:NH1   | 48:WA:73:A:N7     | 2.45                     | 0.63              |
| 15:O:161:ALA:HB2   | 48:WA:1599:G:H5'  | 1.81                     | 0.63              |
| 51:ZA:1521:C:OP2   | 70:SB:136:THR:OG1 | 2.16                     | 0.63              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 16:P:65:ARG:NH1   | 48:WA:1504:G:OP1  | 2.32                     | 0.63              |
| 51:ZA:925:G:H1    | 51:ZA:1017:U:H3   | 1.47                     | 0.63              |
| 5:E:61:ARG:HB2    | 48:WA:1243:C:H5'' | 1.81                     | 0.63              |
| 8:H:43:VAL:HG12   | 8:H:59:LYS:HD3    | 1.78                     | 0.63              |
| 1:A:128:ARG:NH1   | 48:WA:3683:G:OP2  | 2.32                     | 0.63              |
| 33:GA:66:LYS:HD3  | 50:YA:96:C:H5''   | 1.80                     | 0.63              |
| 48:WA:2505:G:O2'  | 48:WA:2507:C:N4   | 2.32                     | 0.63              |
| 58:GB:164:LYS:HG2 | 58:GB:165:GLU:HG3 | 1.80                     | 0.63              |
| 50:YA:67:U:H2'    | 50:YA:68:G:H8     | 1.62                     | 0.62              |
| 51:ZA:43:U:OP2    | 51:ZA:485:A:N6    | 2.30                     | 0.62              |
| 7:G:111:PRO:HD2   | 7:G:114:ILE:HD12  | 1.81                     | 0.62              |
| 21:U:43:LYS:HD3   | 21:U:62:MET:HE2   | 1.81                     | 0.62              |
| 48:WA:67:C:OP2    | 48:WA:312:G:N2    | 2.31                     | 0.62              |
| 48:WA:300:A:H2'   | 48:WA:301:G:H8    | 1.63                     | 0.62              |
| 48:WA:2491:C:O2'  | 48:WA:2493:C:N3   | 2.32                     | 0.62              |
| 53:BB:122:GLU:O   | 53:BB:165:ARG:NH1 | 2.32                     | 0.62              |
| 16:P:82:VAL:HG12  | 16:P:84:GLY:H     | 1.63                     | 0.62              |
| 48:WA:20:U:H3'    | 48:WA:21:G:H8     | 1.64                     | 0.62              |
| 75:XB:68:LYS:HE2  | 82:EC:82:VAL:HG22 | 1.80                     | 0.62              |
| 1:A:116:LEU:HB3   | 1:A:126:LEU:HB2   | 1.82                     | 0.62              |
| 1:A:179:ILE:HG23  | 1:A:184:ARG:HB2   | 1.81                     | 0.62              |
| 2:B:234:ARG:NH2   | 48:WA:4568:U:O2'  | 2.33                     | 0.62              |
| 16:P:65:ARG:NH2   | 48:WA:1461:A:OP1  | 2.32                     | 0.62              |
| 26:Z:72:THR:HG22  | 26:Z:110:LYS:HB3  | 1.81                     | 0.62              |
| 48:WA:2460:C:H1'  | 48:WA:3673:G:H21  | 1.65                     | 0.62              |
| 62:KB:27:VAL:HG13 | 62:KB:43:LEU:HD13 | 1.81                     | 0.62              |
| 10:J:99:PHE:O     | 10:J:159:LYS:NZ   | 2.32                     | 0.62              |
| 30:DA:36:ARG:NH1  | 48:WA:1663:C:OP1  | 2.33                     | 0.62              |
| 51:ZA:1228:A:H2'  | 51:ZA:1229:G:C8   | 2.35                     | 0.62              |
| 1:A:117:GLU:OE2   | 1:A:163:ARG:NH1   | 2.32                     | 0.62              |
| 49:XA:28:C:H1'    | 49:XA:54:A:H61    | 1.64                     | 0.62              |
| 51:ZA:1612:G:OP1  | 67:PB:18:ARG:NH2  | 2.33                     | 0.62              |
| 48:WA:2603:A:N6   | 48:WA:2746:A:OP2  | 2.32                     | 0.62              |
| 51:ZA:616:A:OP1   | 75:XB:68:LYS:NZ   | 2.31                     | 0.62              |
| 38:LA:88:LYS:NZ   | 48:WA:4487:C:O2'  | 2.33                     | 0.62              |
| 51:ZA:163:U:OP2   | 58:GB:87:ARG:NH2  | 2.30                     | 0.62              |
| 14:N:49:ARG:NH1   | 48:WA:1932:U:OP2  | 2.31                     | 0.61              |
| 5:E:164:ARG:NH1   | 12:L:106:ASP:OD2  | 2.32                     | 0.61              |
| 51:ZA:429:C:O2'   | 51:ZA:811:A:N1    | 2.33                     | 0.61              |
| 51:ZA:1259:A:N6   | 51:ZA:1519:U:OP1  | 2.33                     | 0.61              |
| 51:ZA:1652:G:H1   | 51:ZA:1672:U:H3   | 1.47                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 58:GB:2:LYS:HB3   | 58:GB:15:LEU:HD11 | 1.82                     | 0.61              |
| 61:JB:136:ARG:NH1 | 61:JB:159:PHE:O   | 2.32                     | 0.61              |
| 6:F:176:ARG:NH1   | 48:WA:2103:A:N7   | 2.49                     | 0.61              |
| 6:F:218:GLY:O     | 6:F:245:ARG:NH2   | 2.34                     | 0.61              |
| 51:ZA:1286:G:N2   | 51:ZA:1312:G:O2'  | 2.31                     | 0.61              |
| 30:DA:36:ARG:NH2  | 48:WA:2324:G:OP1  | 2.33                     | 0.61              |
| 51:ZA:16:G:H5'    | 51:ZA:669:A:H61   | 1.64                     | 0.61              |
| 81:DC:17:GLY:O    | 81:DC:27:ARG:NH1  | 2.33                     | 0.61              |
| 51:ZA:165:G:N2    | 51:ZA:165:G:OP2   | 2.32                     | 0.61              |
| 51:ZA:581:U:OP1   | 61:JB:133:ARG:NH2 | 2.33                     | 0.61              |
| 51:ZA:954:U:O2    | 66:OB:55:ARG:NH2  | 2.33                     | 0.61              |
| 51:ZA:1004:U:H2'  | 51:ZA:1005:G:H8   | 1.66                     | 0.61              |
| 51:ZA:1227:G:N2   | 51:ZA:1635:C:O2'  | 2.33                     | 0.61              |
| 65:NB:99:ARG:NH2  | 65:NB:119:GLU:OE2 | 2.34                     | 0.61              |
| 17:Q:172:ARG:HH12 | 51:ZA:908:A:H5''  | 1.65                     | 0.61              |
| 42:PA:67:ARG:NH1  | 48:WA:667:G:OP2   | 2.34                     | 0.61              |
| 5:E:156:LEU:HD11  | 5:E:198:ILE:HG13  | 1.82                     | 0.61              |
| 7:G:185:ARG:NH1   | 48:WA:119:G:OP1   | 2.34                     | 0.61              |
| 9:I:203:ARG:NH1   | 49:XA:105:C:OP2   | 2.33                     | 0.61              |
| 11:K:35:ARG:NH1   | 48:WA:105:A:O2'   | 2.34                     | 0.61              |
| 42:PA:65:LYS:O    | 42:PA:102:TYR:OH  | 2.18                     | 0.61              |
| 44:SA:33:U:OP2    | 68:QB:172:ARG:NH2 | 2.34                     | 0.61              |
| 48:WA:35:U:O2'    | 48:WA:1527:A:N1   | 2.34                     | 0.61              |
| 48:WA:2779:G:H5'' | 48:WA:2780:G:H5'  | 1.82                     | 0.61              |
| 48:WA:3879:A:N3   | 48:WA:4403:G:O2'  | 2.30                     | 0.61              |
| 51:ZA:1115:U:H1'  | 51:ZA:1116:C:H2'  | 1.83                     | 0.61              |
| 80:CC:17:VAL:HA   | 80:CC:30:VAL:HG23 | 1.83                     | 0.61              |
| 88:HC:426:VAL:HB  | 88:HC:434:ALA:HB3 | 1.82                     | 0.61              |
| 20:T:113:ARG:NH2  | 48:WA:2704:C:O3'  | 2.33                     | 0.61              |
| 29:CA:39:LYS:HG3  | 29:CA:40:LYS:HG2  | 1.83                     | 0.61              |
| 14:N:116:LYS:HE3  | 18:R:169:THR:HG21 | 1.82                     | 0.60              |
| 41:OA:4:ARG:NH1   | 48:WA:1556:A:OP2  | 2.33                     | 0.60              |
| 68:QB:156:LYS:NZ  | 68:QB:160:GLY:O   | 2.33                     | 0.60              |
| 11:K:54:PRO:HG2   | 11:K:56:ARG:HH12  | 1.66                     | 0.60              |
| 16:P:16:LYS:O     | 16:P:33:ARG:NH2   | 2.34                     | 0.60              |
| 48:WA:4747:G:H1   | 48:WA:4957:A:H61  | 1.47                     | 0.60              |
| 70:SB:101:ASN:O   | 70:SB:105:ASN:ND2 | 2.32                     | 0.60              |
| 25:Y:48:ARG:NH2   | 48:WA:2578:G:OP1  | 2.34                     | 0.60              |
| 35:IA:52:LYS:NZ   | 48:WA:364:G:O6    | 2.33                     | 0.60              |
| 48:WA:2337:C:H2'  | 48:WA:2338:G:H8   | 1.65                     | 0.60              |
| 52:AB:36:GLN:O    | 52:AB:53:ARG:NH1  | 2.34                     | 0.60              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 84:GC:4:GLN:HB3    | 84:GC:313:THR:HB  | 1.83                     | 0.60              |
| 51:ZA:1418:C:H5'   | 51:ZA:1420:G:H21  | 1.65                     | 0.60              |
| 48:WA:2522:C:H2'   | 48:WA:2523:G:H8   | 1.66                     | 0.60              |
| 51:ZA:1228:A:H2'   | 51:ZA:1229:G:H8   | 1.66                     | 0.60              |
| 5:E:159:ARG:NH1    | 48:WA:4942:C:OP1  | 2.33                     | 0.60              |
| 33:GA:31:LEU:HB3   | 33:GA:47:ILE:HG22 | 1.82                     | 0.60              |
| 61:JB:131:ARG:NH1  | 61:JB:143:ASN:OD1 | 2.35                     | 0.60              |
| 13:M:192:TRP:NE1   | 48:WA:48:G:OP1    | 2.32                     | 0.60              |
| 22:V:93:LYS:O      | 22:V:101:ARG:NH2  | 2.34                     | 0.60              |
| 26:Z:65:ARG:NH2    | 48:WA:86:U:O2'    | 2.34                     | 0.60              |
| 48:WA:262:G:H2'    | 48:WA:263:G:C8    | 2.37                     | 0.60              |
| 51:ZA:1528:G:O2'   | 51:ZA:1666:C:OP1  | 2.20                     | 0.60              |
| 51:ZA:1568:C:O2    | 51:ZA:1627:C:O2'  | 2.19                     | 0.60              |
| 84:GC:174:VAL:HB   | 84:GC:188:HIS:HB2 | 1.83                     | 0.60              |
| 51:ZA:1566:G:N7    | 71:TB:101:ARG:NH2 | 2.49                     | 0.60              |
| 51:ZA:1677:U:OP1   | 57:FB:71:ARG:NH2  | 2.35                     | 0.60              |
| 7:G:170:ARG:NH2    | 48:WA:119:G:O6    | 2.33                     | 0.60              |
| 9:I:54:SER:HB2     | 9:I:135:ILE:HD11  | 1.84                     | 0.60              |
| 30:DA:8:VAL:HG22   | 30:DA:10:PRO:HD3  | 1.82                     | 0.60              |
| 48:WA:1973:U:O2    | 86:b:41:GLN:NE2   | 2.34                     | 0.60              |
| 48:WA:2640:G:H1    | 48:WA:2699:A:H61  | 1.47                     | 0.60              |
| 67:PB:121:ILE:HG22 | 70:SB:120:HIS:HD2 | 1.66                     | 0.60              |
| 48:WA:1857:G:O6    | 48:WA:1882:G:N2   | 2.35                     | 0.60              |
| 48:WA:4276:A:H2'   | 48:WA:4277:G:H8   | 1.66                     | 0.60              |
| 70:SB:50:ILE:HD11  | 70:SB:63:GLU:HB3  | 1.84                     | 0.60              |
| 51:ZA:1550:G:H3'   | 51:ZA:1579:A:H61  | 1.67                     | 0.59              |
| 75:XB:91:LEU:HB3   | 82:EC:82:VAL:HG11 | 1.83                     | 0.59              |
| 22:V:61:LYS:NZ     | 48:WA:5040:A:OP1  | 2.35                     | 0.59              |
| 45:TA:15:G:N2      | 45:TA:48:C:O2     | 2.36                     | 0.59              |
| 51:ZA:1261:C:O2    | 81:DC:10:HIS:NE2  | 2.29                     | 0.59              |
| 51:ZA:1286:G:OP1   | 83:FC:99:LYS:NZ   | 2.35                     | 0.59              |
| 51:ZA:1447:G:OP1   | 72:UB:85:HIS:ND1  | 2.35                     | 0.59              |
| 51:ZA:197:U:O4     | 51:ZA:202:G:O6    | 2.19                     | 0.59              |
| 51:ZA:1447:G:OP1   | 72:UB:87:ARG:NH2  | 2.35                     | 0.59              |
| 2:B:385:LYS:NZ     | 48:WA:5004:U:OP2  | 2.35                     | 0.59              |
| 7:G:210:ILE:HA     | 7:G:254:THR:HG22  | 1.84                     | 0.59              |
| 48:WA:5055:U:OP1   | 48:WA:5056:C:N4   | 2.35                     | 0.59              |
| 51:ZA:1015:U:O2'   | 65:NB:55:ARG:NH1  | 2.36                     | 0.59              |
| 5:E:265:LYS:NZ     | 48:WA:4935:C:OP2  | 2.34                     | 0.59              |
| 28:BA:36:LYS:NZ    | 48:WA:2659:G:OP2  | 2.35                     | 0.59              |
| 48:WA:1392:G:N2    | 48:WA:1395:G:OP2  | 2.34                     | 0.59              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 48:WA:4476:A:OP2   | 48:WA:4478:C:N4    | 2.35                     | 0.59              |
| 48:WA:4920:C:H2'   | 48:WA:4921:G:H8    | 1.68                     | 0.59              |
| 51:ZA:1513:C:OP1   | 81:DC:12:ARG:NH1   | 2.35                     | 0.59              |
| 57:FB:114:ASN:OD1  | 57:FB:118:ASN:ND2  | 2.35                     | 0.59              |
| 3:C:110:ARG:O      | 3:C:113:ARG:NH1    | 2.35                     | 0.59              |
| 7:G:282:ARG:NH2    | 7:G:285:GLU:OE1    | 2.36                     | 0.59              |
| 24:X:55:VAL:HG12   | 24:X:106:ILE:HA    | 1.84                     | 0.59              |
| 38:LA:92:THR:HG22  | 38:LA:94:ASN:H     | 1.67                     | 0.59              |
| 59:HB:408:VAL:HG13 | 59:HB:425:PHE:HB2  | 1.83                     | 0.59              |
| 84:GC:202:PRO:HG2  | 84:GC:243:PRO:HA   | 1.85                     | 0.59              |
| 56:EB:87:MET:HE1   | 56:EB:236:ILE:HG21 | 1.84                     | 0.59              |
| 24:X:34:LEU:HD23   | 24:X:38:LEU:HB3    | 1.85                     | 0.59              |
| 49:XA:53:U:H4'     | 49:XA:54:A:H5'     | 1.85                     | 0.59              |
| 51:ZA:24:C:OP1     | 61:JB:11:LYS:NZ    | 2.32                     | 0.59              |
| 51:ZA:1092:G:OP1   | 65:NB:2:GLY:N      | 2.36                     | 0.59              |
| 51:ZA:1373:C:O2'   | 69:RB:10:LYS:NZ    | 2.30                     | 0.59              |
| 6:F:104:VAL:HG13   | 6:F:135:VAL:HG12   | 1.85                     | 0.59              |
| 34:HA:48:CYS:SG    | 34:HA:49:GLY:N     | 2.76                     | 0.59              |
| 48:WA:3863:A:H2'   | 48:WA:3864:A:H8    | 1.68                     | 0.59              |
| 51:ZA:1758:G:H2'   | 51:ZA:1759:G:C8    | 2.38                     | 0.59              |
| 65:NB:136:PRO:HG2  | 65:NB:139:TRP:HB2  | 1.83                     | 0.59              |
| 70:SB:23:ARG:NH2   | 77:ZB:46:ASN:O     | 2.34                     | 0.59              |
| 2:B:258:HIS:NE2    | 48:WA:3880:C:O2    | 2.36                     | 0.59              |
| 11:K:116:ARG:NH2   | 11:K:155:MET:O     | 2.36                     | 0.59              |
| 13:M:157:LYS:O     | 13:M:162:ARG:NH1   | 2.36                     | 0.59              |
| 48:WA:1972:A:H5'   | 86:b:37:SER:HB3    | 1.84                     | 0.59              |
| 48:WA:2555:A:N6    | 48:WA:2767:A:OP2   | 2.35                     | 0.59              |
| 61:JB:127:ARG:HD3  | 82:EC:104:ARG:HD3  | 1.83                     | 0.59              |
| 4:D:83:LEU:HB3     | 4:D:88:VAL:HB      | 1.84                     | 0.58              |
| 9:I:4:ARG:NH1      | 48:WA:1868:U:OP1   | 2.32                     | 0.58              |
| 14:N:54:TYR:OH     | 14:N:73:PHE:O      | 2.21                     | 0.58              |
| 17:Q:105:LEU:HD23  | 17:Q:138:LEU:HD23  | 1.84                     | 0.58              |
| 48:WA:4994:G:H2'   | 48:WA:4995:G:H8    | 1.68                     | 0.58              |
| 51:ZA:106:C:H2'    | 51:ZA:107:A:H8     | 1.68                     | 0.58              |
| 51:ZA:688:U:OP1    | 59:HB:354:ARG:NH2  | 2.36                     | 0.58              |
| 51:ZA:1587:G:H21   | 71:TB:77:LYS:HD3   | 1.67                     | 0.58              |
| 51:ZA:1617:G:N1    | 51:ZA:1620:A:OP2   | 2.34                     | 0.58              |
| 16:P:22:ASP:OD1    | 16:P:22:ASP:N      | 2.35                     | 0.58              |
| 55:DB:257:PRO:HB2  | 84:GC:190:GLY:HA2  | 1.85                     | 0.58              |
| 59:HB:268:LEU:O    | 59:HB:272:SER:CB   | 2.51                     | 0.58              |
| 84:GC:107:ASP:OD2  | 84:GC:125:ARG:NH1  | 2.36                     | 0.58              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 14:N:89:PRO:HD3    | 48:WA:1916:C:H4'   | 1.85                     | 0.58              |
| 17:Q:108:ARG:NH2   | 48:WA:2901:C:OP1   | 2.34                     | 0.58              |
| 21:U:15:ARG:NH2    | 48:WA:4675:U:OP2   | 2.36                     | 0.58              |
| 48:WA:2601:G:N2    | 48:WA:2749:U:O4    | 2.35                     | 0.58              |
| 48:WA:2737:G:H2'   | 48:WA:2738:G:H8    | 1.67                     | 0.58              |
| 48:WA:3850:U:H2'   | 48:WA:3851:A:H8    | 1.67                     | 0.58              |
| 51:ZA:183:G:O2'    | 51:ZA:184:G:O4'    | 2.21                     | 0.58              |
| 57:FB:35:LEU:HD22  | 57:FB:117:ILE:HD13 | 1.85                     | 0.58              |
| 57:FB:50:PRO:HG2   | 57:FB:90:VAL:HG22  | 1.85                     | 0.58              |
| 61:JB:137:VAL:HG22 | 61:JB:157:ILE:HG12 | 1.85                     | 0.58              |
| 68:QB:158:PHE:O    | 68:QB:166:ARG:NH1  | 2.36                     | 0.58              |
| 88:HC:352:GLN:HB2  | 88:HC:393:PHE:HB2  | 1.85                     | 0.58              |
| 3:C:204:ARG:NH1    | 3:C:205:ARG:O      | 2.36                     | 0.58              |
| 5:E:185:ASN:ND2    | 5:E:274:LEU:O      | 2.34                     | 0.58              |
| 6:F:146:LEU:O      | 6:F:150:ASN:ND2    | 2.37                     | 0.58              |
| 9:I:152:LEU:HB3    | 9:I:165:ILE:HD12   | 1.85                     | 0.58              |
| 19:S:108:ARG:NH1   | 48:WA:1839:A:OP1   | 2.37                     | 0.58              |
| 23:W:110:LYS:HG3   | 23:W:121:VAL:HB    | 1.86                     | 0.58              |
| 40:NA:2:VAL:N      | 40:NA:90:HIS:O     | 2.36                     | 0.58              |
| 74:WB:52:ILE:HG22  | 74:WB:61:ILE:HG12  | 1.84                     | 0.58              |
| 15:O:160:ARG:NH2   | 48:WA:1599:G:OP1   | 2.37                     | 0.58              |
| 48:WA:1797:A:N3    | 49:XA:79:U:O2'     | 2.37                     | 0.58              |
| 56:EB:66:MET:SD    | 56:EB:78:THR:OG1   | 2.62                     | 0.58              |
| 88:HC:378:LYS:HD2  | 88:HC:391:PRO:HB3  | 1.86                     | 0.58              |
| 2:B:11:HIS:NE2     | 48:WA:4460:C:OP1   | 2.36                     | 0.58              |
| 7:G:96:GLN:O       | 48:WA:4126:G:N2    | 2.37                     | 0.58              |
| 7:G:276:ARG:HG3    | 7:G:280:ASN:HB2    | 1.85                     | 0.58              |
| 24:X:30:MET:HB3    | 24:X:101:PRO:HG2   | 1.84                     | 0.58              |
| 48:WA:2409:G:OP2   | 48:WA:2409:G:N2    | 2.34                     | 0.58              |
| 48:WA:3892:A:N6    | 48:WA:4572:G:O2'   | 2.36                     | 0.58              |
| 56:EB:112:HIS:NE2  | 56:EB:237:SER:O    | 2.37                     | 0.58              |
| 2:B:20:LYS:HD3     | 48:WA:4719:A:H4'   | 1.86                     | 0.58              |
| 16:P:67:ILE:HD12   | 16:P:96:PRO:HD2    | 1.85                     | 0.58              |
| 31:EA:43:LEU:O     | 31:EA:109:ARG:NH1  | 2.37                     | 0.58              |
| 32:FA:29:ARG:NH1   | 48:WA:2524:G:OP1   | 2.36                     | 0.58              |
| 48:WA:2320:G:N2    | 48:WA:2323:G:OP2   | 2.29                     | 0.58              |
| 48:WA:2577:U:O2    | 48:WA:2760:G:N2    | 2.35                     | 0.58              |
| 67:PB:56:LEU:HD23  | 67:PB:83:MET:HE3   | 1.84                     | 0.58              |
| 73:VB:16:LYS:HG2   | 73:VB:23:ILE:HG22  | 1.85                     | 0.58              |
| 84:GC:18:VAL:HA    | 84:GC:35:SER:HA    | 1.85                     | 0.58              |
| 48:WA:1255:G:H1    | 48:WA:1262:G:H22   | 1.52                     | 0.58              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 48:WA:4090:C:H2'  | 48:WA:4091:G:H8    | 1.69                     | 0.58              |
| 51:ZA:1353:A:OP1  | 52:AB:139:TYR:OH   | 2.16                     | 0.58              |
| 13:M:96:ARG:NH2   | 13:M:104:GLU:OE1   | 2.37                     | 0.57              |
| 48:WA:4596:U:H2'  | 48:WA:4597:G:H8    | 1.69                     | 0.57              |
| 51:ZA:1271:C:OP1  | 83:FC:90:LYS:NZ    | 2.37                     | 0.57              |
| 51:ZA:1472:C:H42  | 51:ZA:1476:A:N6    | 1.97                     | 0.57              |
| 70:SB:34:LYS:HB3  | 70:SB:100:ALA:HA   | 1.86                     | 0.57              |
| 88:HC:360:VAL:HA  | 88:HC:369:ALA:HA   | 1.86                     | 0.57              |
| 2:B:317:LEU:HB2   | 2:B:372:SER:HB2    | 1.86                     | 0.57              |
| 48:WA:1446:G:N2   | 48:WA:2113:U:O2    | 2.30                     | 0.57              |
| 48:WA:2772:C:H2'  | 48:WA:2773:G:H8    | 1.68                     | 0.57              |
| 51:ZA:486:A:H1'   | 51:ZA:513:G:H22    | 1.69                     | 0.57              |
| 51:ZA:1513:C:H2'  | 51:ZA:1514:G:H8    | 1.69                     | 0.57              |
| 74:WB:11:LEU:HD12 | 74:WB:74:VAL:HG22  | 1.85                     | 0.57              |
| 48:WA:2411:U:H4'  | 48:WA:2430:A:H4'   | 1.87                     | 0.57              |
| 51:ZA:1562:C:H2'  | 51:ZA:1563:G:H8    | 1.69                     | 0.57              |
| 56:EB:151:ASP:HB3 | 56:EB:154:ILE:HG12 | 1.86                     | 0.57              |
| 5:E:129:LEU:O     | 48:WA:965:A:N6     | 2.37                     | 0.57              |
| 27:AA:99:ILE:O    | 27:AA:109:ARG:NH1  | 2.37                     | 0.57              |
| 30:DA:109:LYS:NZ  | 30:DA:128:ARG:O    | 2.34                     | 0.57              |
| 48:WA:2377:A:H2'  | 48:WA:2378:A:H8    | 1.68                     | 0.57              |
| 51:ZA:4:C:H4'     | 54:CB:207:ALA:HB2  | 1.86                     | 0.57              |
| 51:ZA:453:C:O2'   | 58:GB:92:ARG:O     | 2.22                     | 0.57              |
| 51:ZA:617:G:H4'   | 75:XB:88:ASP:HB2   | 1.85                     | 0.57              |
| 63:LB:13:GLN:HE22 | 63:LB:35:ARG:HG3   | 1.70                     | 0.57              |
| 16:P:14:ARG:NH2   | 48:WA:2085:C:OP2   | 2.37                     | 0.57              |
| 49:XA:92:C:H2'    | 49:XA:93:G:H8      | 1.68                     | 0.57              |
| 54:CB:69:LEU:HG   | 54:CB:273:LEU:HD21 | 1.87                     | 0.57              |
| 79:BC:34:ASP:HB2  | 79:BC:82:LYS:HD2   | 1.85                     | 0.57              |
| 4:D:33:ARG:NE     | 49:XA:7:G:OP1      | 2.36                     | 0.57              |
| 48:WA:4910:G:O2'  | 48:WA:4915:G:N2    | 2.38                     | 0.57              |
| 51:ZA:608:C:O4'   | 82:EC:131:ASN:ND2  | 2.37                     | 0.57              |
| 48:WA:158:A:N1    | 48:WA:276:C:O2'    | 2.35                     | 0.57              |
| 67:PB:123:TYR:OH  | 70:SB:124:ARG:NH1  | 2.36                     | 0.57              |
| 42:PA:98:ARG:NH2  | 48:WA:2264:G:OP2   | 2.37                     | 0.57              |
| 48:WA:4:G:H2'     | 48:WA:5:A:H8       | 1.69                     | 0.57              |
| 48:WA:2649:A:H62  | 48:WA:2688:G:H8    | 1.51                     | 0.57              |
| 51:ZA:1565:C:OP2  | 71:TB:101:ARG:NH1  | 2.37                     | 0.57              |
| 59:HB:245:LYS:NZ  | 59:HB:269:GLU:OE2  | 2.35                     | 0.57              |
| 88:HC:281:ALA:HB2 | 88:HC:334:PRO:HB2  | 1.87                     | 0.57              |
| 10:J:87:LEU:HD12  | 10:J:92:TYR:HA     | 1.86                     | 0.57              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 14:N:72:HIS:N      | 48:WA:4588:G:OP1   | 2.38                     | 0.57              |
| 14:N:74:ARG:N      | 48:WA:4587:U:OP1   | 2.36                     | 0.57              |
| 19:S:87:LYS:NZ     | 48:WA:4302:U:OP1   | 2.35                     | 0.57              |
| 21:U:13:LYS:NZ     | 21:U:59:ASP:OD1    | 2.37                     | 0.57              |
| 56:EB:162:ILE:HG22 | 56:EB:169:ILE:HA   | 1.87                     | 0.57              |
| 70:SB:98:VAL:HG11  | 70:SB:106:LYS:HG3  | 1.86                     | 0.57              |
| 37:KA:48:LYS:NZ    | 48:WA:2793:C:OP1   | 2.32                     | 0.57              |
| 40:NA:98:LYS:HD2   | 48:WA:4235:A:H4'   | 1.86                     | 0.57              |
| 51:ZA:612:U:O2'    | 82:EC:84:LYS:NZ    | 2.38                     | 0.57              |
| 51:ZA:1477:U:OP2   | 69:RB:3:ARG:NH2    | 2.38                     | 0.57              |
| 64:MB:52:LEU:HD23  | 64:MB:76:LEU:HD11  | 1.87                     | 0.57              |
| 1:A:6:ARG:HH12     | 1:A:199:VAL:H      | 1.53                     | 0.56              |
| 9:I:77:VAL:HG23    | 9:I:82:LYS:HA      | 1.87                     | 0.56              |
| 48:WA:4956:G:H2'   | 48:WA:4957:A:H8    | 1.70                     | 0.56              |
| 65:NB:24:THR:O     | 65:NB:27:LYS:NZ    | 2.35                     | 0.56              |
| 65:NB:33:VAL:HG21  | 65:NB:66:VAL:HG11  | 1.87                     | 0.56              |
| 2:B:5:LYS:NZ       | 48:WA:4503:U:OP1   | 2.38                     | 0.56              |
| 31:EA:54:LYS:HE3   | 48:WA:4750:U:H5''  | 1.86                     | 0.56              |
| 38:LA:96:ARG:NH2   | 48:WA:4475:A:O2'   | 2.38                     | 0.56              |
| 48:WA:2899:G:H2'   | 48:WA:2900:G:H8    | 1.70                     | 0.56              |
| 51:ZA:1419:C:OP2   | 51:ZA:1420:G:N2    | 2.37                     | 0.56              |
| 51:ZA:1432:U:H2'   | 51:ZA:1438:A:H8    | 1.69                     | 0.56              |
| 69:RB:95:ILE:HD11  | 69:RB:118:GLN:HB2  | 1.86                     | 0.56              |
| 4:D:88:VAL:HA      | 4:D:239:MET:HE3    | 1.86                     | 0.56              |
| 11:K:48:PRO:HG3    | 33:GA:118:LYS:HE3  | 1.87                     | 0.56              |
| 12:L:11:ARG:NH1    | 12:L:58:THR:O      | 2.37                     | 0.56              |
| 21:U:41:SER:HG     | 48:WA:4509:A:HO2'  | 1.44                     | 0.56              |
| 36:JA:35:LYS:NZ    | 48:WA:2695:G:OP1   | 2.30                     | 0.56              |
| 44:SA:38:C:O2'     | 51:ZA:1058:A:OP1   | 2.23                     | 0.56              |
| 51:ZA:527:C:O2'    | 61:JB:121:LYS:NZ   | 2.37                     | 0.56              |
| 51:ZA:1531:A:OP1   | 71:TB:84:ARG:NH2   | 2.37                     | 0.56              |
| 51:ZA:1858:G:OP2   | 66:OB:146:ARG:NH2  | 2.33                     | 0.56              |
| 54:CB:68:ARG:NH1   | 54:CB:72:ASP:OD1   | 2.39                     | 0.56              |
| 56:EB:191:ARG:HH11 | 56:EB:245:ARG:HH21 | 1.52                     | 0.56              |
| 70:SB:89:ASP:OD1   | 70:SB:94:LYS:N     | 2.38                     | 0.56              |
| 70:SB:124:ARG:HB2  | 70:SB:131:VAL:HG13 | 1.88                     | 0.56              |
| 78:AC:87:ARG:NH2   | 78:AC:91:ALA:O     | 2.38                     | 0.56              |
| 83:FC:126:CYS:HB2  | 83:FC:144:CYS:HB2  | 1.86                     | 0.56              |
| 2:B:276:HIS:ND1    | 48:WA:4718:C:OP1   | 2.37                     | 0.56              |
| 26:Z:125:LYS:HG2   | 26:Z:145:VAL:HB    | 1.87                     | 0.56              |
| 46:UA:59:A:N7      | 46:UA:60:A:N6      | 2.53                     | 0.56              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 48:WA:62:A:N3     | 48:WA:77:U:O2'     | 2.30                     | 0.56              |
| 51:ZA:1745:A:H62  | 51:ZA:1789:G:H21   | 1.53                     | 0.56              |
| 59:HB:355:PRO:HG2 | 59:HB:358:ARG:HG2  | 1.86                     | 0.56              |
| 64:MB:51:VAL:O    | 64:MB:108:CYS:HA   | 2.06                     | 0.56              |
| 13:M:90:ASN:ND2   | 48:WA:3930:A:OP1   | 2.38                     | 0.56              |
| 19:S:71:ALA:HB3   | 48:WA:4315:A:H4'   | 1.88                     | 0.56              |
| 21:U:13:LYS:HD2   | 21:U:128:LEU:HD11  | 1.88                     | 0.56              |
| 46:UA:74:C:H3'    | 46:UA:75:C:H5''    | 1.87                     | 0.56              |
| 48:WA:369:G:N2    | 48:WA:372:A:OP2    | 2.31                     | 0.56              |
| 48:WA:992:C:O2    | 48:WA:1076:G:N2    | 2.38                     | 0.56              |
| 48:WA:1095:G:H2'  | 48:WA:1096:G:H8    | 1.70                     | 0.56              |
| 48:WA:4274:G:OP2  | 48:WA:4274:G:N2    | 2.39                     | 0.56              |
| 51:ZA:677:G:N2    | 51:ZA:1028:A:H62   | 2.00                     | 0.56              |
| 51:ZA:1147:C:OP1  | 78:AC:6:ARG:NH1    | 2.36                     | 0.56              |
| 51:ZA:1156:U:O4   | 54:CB:194:ARG:NH1  | 2.38                     | 0.56              |
| 51:ZA:1270:G:O2'  | 51:ZA:1299:A:N6    | 2.34                     | 0.56              |
| 51:ZA:1613:G:OP1  | 70:SB:88:LYS:NZ    | 2.38                     | 0.56              |
| 56:EB:100:ARG:HB2 | 56:EB:114:ILE:HD13 | 1.87                     | 0.56              |
| 71:TB:22:LEU:HG   | 71:TB:28:LEU:HD21  | 1.87                     | 0.56              |
| 76:YB:82:ALA:O    | 76:YB:86:GLU:HB2   | 2.05                     | 0.56              |
| 86:b:53:VAL:HG12  | 86:b:89:VAL:HG12   | 1.88                     | 0.56              |
| 37:KA:13:LEU:HD22 | 48:WA:2409:G:H2'   | 1.87                     | 0.56              |
| 10:J:146:ARG:NH1  | 49:XA:27:G:OP1     | 2.39                     | 0.56              |
| 11:K:140:SER:OG   | 11:K:143:GLU:OE1   | 2.22                     | 0.56              |
| 12:L:80:ALA:O     | 12:L:85:LYS:NZ     | 2.35                     | 0.56              |
| 13:M:114:ARG:HE   | 13:M:137:PRO:HG3   | 1.70                     | 0.56              |
| 13:M:116:LEU:HD22 | 13:M:135:ILE:HD11  | 1.87                     | 0.56              |
| 48:WA:1213:C:H2'  | 48:WA:1214:G:H8    | 1.69                     | 0.56              |
| 51:ZA:126:G:H1'   | 51:ZA:181:A:H1'    | 1.87                     | 0.56              |
| 68:QB:79:GLU:OE1  | 68:QB:111:ARG:NH1  | 2.38                     | 0.56              |
| 8:H:128:MET:HE2   | 8:H:134:CYS:HB2    | 1.88                     | 0.56              |
| 25:Y:3:LYS:O      | 25:Y:6:LYS:NZ      | 2.39                     | 0.56              |
| 48:WA:1804:A:H5'' | 48:WA:1805:G:H5'   | 1.87                     | 0.56              |
| 48:WA:1886:C:H2'  | 48:WA:1887:G:H8    | 1.71                     | 0.56              |
| 48:WA:3809:A:HO2' | 51:ZA:1816:G:HO2'  | 1.54                     | 0.56              |
| 59:HB:244:ALA:HB3 | 59:HB:262:SER:HB2  | 1.87                     | 0.56              |
| 20:T:25:CYS:HB2   | 20:T:28:PRO:HG2    | 1.88                     | 0.56              |
| 25:Y:100:VAL:HG13 | 25:Y:106:LEU:HB3   | 1.88                     | 0.56              |
| 32:FA:6:THR:HG22  | 48:WA:2402:G:H21   | 1.71                     | 0.56              |
| 48:WA:4637:A:H2   | 48:WA:4665:G:H21   | 1.52                     | 0.56              |
| 51:ZA:928:G:H2'   | 51:ZA:929:G:C8     | 2.41                     | 0.56              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 51:ZA:1351:G:H1   | 51:ZA:1360:U:H3    | 1.54                     | 0.56              |
| 53:BB:82:ARG:NH2  | 53:BB:191:ASP:OD1  | 2.39                     | 0.56              |
| 57:FB:49:LEU:HD11 | 68:QB:75:TYR:HB3   | 1.87                     | 0.56              |
| 76:YB:34:THR:HG23 | 76:YB:69:THR:HG21  | 1.88                     | 0.56              |
| 1:A:117:GLU:O     | 1:A:162:ASN:ND2    | 2.38                     | 0.56              |
| 26:Z:132:ARG:NH1  | 48:WA:1470:C:OP1   | 2.39                     | 0.56              |
| 27:AA:56:LYS:O    | 27:AA:60:ASN:ND2   | 2.38                     | 0.56              |
| 48:WA:1285:G:N1   | 48:WA:2078:G:OP1   | 2.35                     | 0.56              |
| 48:WA:3918:G:H2'  | 48:WA:3919:A:C8    | 2.41                     | 0.56              |
| 51:ZA:544:G:H2'   | 51:ZA:545:A:H8     | 1.70                     | 0.56              |
| 3:C:321:ASN:OD1   | 48:WA:1282:C:O2'   | 2.23                     | 0.55              |
| 15:O:79:ASP:OD2   | 15:O:85:GLN:NE2    | 2.39                     | 0.55              |
| 48:WA:1334:C:H2'  | 48:WA:1335:A:C8    | 2.42                     | 0.55              |
| 48:WA:1852:A:N3   | 48:WA:2285:G:O2'   | 2.38                     | 0.55              |
| 48:WA:3719:A:N3   | 48:WA:4180:A:O2'   | 2.36                     | 0.55              |
| 48:WA:4241:A:H2'  | 48:WA:4242:G:H8    | 1.71                     | 0.55              |
| 48:WA:4701:U:H1'  | 48:WA:4702:A:H5''  | 1.88                     | 0.55              |
| 51:ZA:64:A:H2     | 51:ZA:83:A:H62     | 1.55                     | 0.55              |
| 51:ZA:1668:U:OP1  | 68:QB:159:GLY:N    | 2.39                     | 0.55              |
| 55:DB:69:GLU:O    | 55:DB:92:ARG:NH2   | 2.39                     | 0.55              |
| 13:M:183:THR:HG22 | 13:M:188:ARG:HB3   | 1.88                     | 0.55              |
| 48:WA:1962:A:H1'  | 86:b:63:LYS:HG2    | 1.87                     | 0.55              |
| 48:WA:4276:A:H2'  | 48:WA:4277:G:C8    | 2.41                     | 0.55              |
| 51:ZA:3:C:O2      | 61:JB:18:ARG:NH1   | 2.39                     | 0.55              |
| 54:CB:94:ILE:HD12 | 54:CB:162:ILE:HD11 | 1.88                     | 0.55              |
| 66:OB:101:GLY:HA3 | 66:OB:134:PRO:HG2  | 1.88                     | 0.55              |
| 1:A:241:ARG:NH1   | 48:WA:3661:G:OP1   | 2.39                     | 0.55              |
| 2:B:329:ASP:OD1   | 2:B:329:ASP:N      | 2.36                     | 0.55              |
| 14:N:130:LYS:HB2  | 14:N:133:ARG:HG2   | 1.88                     | 0.55              |
| 15:O:147:GLN:OE1  | 48:WA:423:G:N2     | 2.33                     | 0.55              |
| 21:U:35:LYS:HB2   | 21:U:67:LYS:HG3    | 1.88                     | 0.55              |
| 29:CA:64:ILE:HG23 | 29:CA:68:LEU:HD23  | 1.88                     | 0.55              |
| 48:WA:1560:A:H2'  | 48:WA:1561:G:H8    | 1.70                     | 0.55              |
| 48:WA:4539:C:H2'  | 48:WA:4540:G:C8    | 2.41                     | 0.55              |
| 66:OB:45:THR:HG22 | 66:OB:52:THR:HA    | 1.88                     | 0.55              |
| 39:MA:23:ARG:NH2  | 48:WA:3809:A:OP1   | 2.38                     | 0.55              |
| 46:UA:21:A:H2'    | 46:UA:22:U:H5''    | 1.88                     | 0.55              |
| 50:YA:67:U:H2'    | 50:YA:68:G:C8      | 2.41                     | 0.55              |
| 51:ZA:874:G:N3    | 59:HB:352:GLN:NE2  | 2.45                     | 0.55              |
| 2:B:224:LYS:NZ    | 48:WA:4669:C:OP1   | 2.35                     | 0.55              |
| 16:P:2:GLY:N      | 48:WA:1900:C:OP1   | 2.40                     | 0.55              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 40:NA:81:ARG:NH2   | 48:WA:4295:U:O2'  | 2.40                     | 0.55              |
| 42:PA:6:GLN:HG3    | 42:PA:44:ILE:HD12 | 1.88                     | 0.55              |
| 51:ZA:1128:C:H2'   | 51:ZA:1129:G:C8   | 2.41                     | 0.55              |
| 52:AB:145:ILE:HG12 | 52:AB:159:ILE:HB  | 1.89                     | 0.55              |
| 7:G:203:LYS:NZ     | 7:G:230:MET:O     | 2.39                     | 0.55              |
| 35:IA:49:TRP:O     | 48:WA:1648:A:O2'  | 2.24                     | 0.55              |
| 48:WA:153:G:H2'    | 48:WA:154:G:H8    | 1.71                     | 0.55              |
| 48:WA:181:C:H2'    | 48:WA:182:G:C8    | 2.42                     | 0.55              |
| 48:WA:308:G:OP2    | 48:WA:308:G:N2    | 2.26                     | 0.55              |
| 48:WA:4110:G:H2'   | 48:WA:4111:G:H8   | 1.70                     | 0.55              |
| 51:ZA:210:U:H2'    | 51:ZA:211:G:H8    | 1.71                     | 0.55              |
| 48:WA:1826:G:H2'   | 48:WA:1827:A:C8   | 2.41                     | 0.55              |
| 48:WA:4176:U:H2'   | 48:WA:4177:G:H8   | 1.70                     | 0.55              |
| 51:ZA:379:C:O2     | 60:IB:5:ARG:NH1   | 2.40                     | 0.55              |
| 51:ZA:527:C:H2'    | 51:ZA:528:A:H8    | 1.71                     | 0.55              |
| 76:YB:82:ALA:O     | 76:YB:86:GLU:CB   | 2.55                     | 0.55              |
| 12:L:35:ARG:NH2    | 18:R:108:GLN:OE1  | 2.36                     | 0.55              |
| 45:TA:49:C:H2'     | 45:TA:50:A:H8     | 1.72                     | 0.55              |
| 48:WA:2507:C:H4'   | 48:WA:2508:G:H5'  | 1.89                     | 0.55              |
| 48:WA:4637:A:OP1   | 48:WA:4638:U:O2'  | 2.24                     | 0.55              |
| 54:CB:60:TRP:O     | 54:CB:71:LYS:NZ   | 2.38                     | 0.55              |
| 1:A:101:VAL:HG22   | 1:A:165:VAL:HG22  | 1.87                     | 0.55              |
| 9:I:101:LYS:NZ     | 9:I:102:MET:O     | 2.37                     | 0.55              |
| 13:M:15:GLN:NE2    | 48:WA:280:G:O6    | 2.40                     | 0.55              |
| 24:X:109:LEU:HD22  | 24:X:115:ARG:HH12 | 1.72                     | 0.55              |
| 48:WA:1183:U:H2'   | 48:WA:1184:G:H8   | 1.72                     | 0.55              |
| 48:WA:1935:G:H2'   | 48:WA:1936:A:C8   | 2.42                     | 0.55              |
| 48:WA:1960:A:O2'   | 48:WA:2027:A:N6   | 2.39                     | 0.55              |
| 48:WA:3601:A:H2'   | 48:WA:3602:G:C8   | 2.42                     | 0.55              |
| 51:ZA:941:C:H2'    | 51:ZA:942:G:H8    | 1.72                     | 0.55              |
| 51:ZA:1240:A:N7    | 67:PB:100:LYS:HB2 | 2.21                     | 0.55              |
| 51:ZA:1529:C:O2'   | 71:TB:87:VAL:O    | 2.25                     | 0.55              |
| 51:ZA:1808:U:H2'   | 51:ZA:1809:A:H8   | 1.71                     | 0.55              |
| 73:VB:15:ARG:NH1   | 73:VB:33:GLN:OE1  | 2.37                     | 0.55              |
| 33:GA:79:LYS:HE3   | 48:WA:136:C:H41   | 1.70                     | 0.55              |
| 48:WA:4423:C:H42   | 48:WA:4477:G:N2   | 2.05                     | 0.55              |
| 51:ZA:1453:C:OP1   | 69:RB:48:ASN:ND2  | 2.40                     | 0.55              |
| 51:ZA:1599:U:OP2   | 77:ZB:46:ASN:ND2  | 2.39                     | 0.55              |
| 74:WB:18:GLU:HG2   | 74:WB:65:LEU:HD13 | 1.89                     | 0.55              |
| 83:FC:141:CYS:HB3  | 83:FC:146:LEU:H   | 1.71                     | 0.55              |
| 4:D:268:ARG:NH1    | 48:WA:1182:C:OP1  | 2.40                     | 0.54              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 10:J:56:THR:HG22  | 10:J:64:ARG:H      | 1.72                     | 0.54              |
| 15:O:150:LYS:O    | 50:YA:13:G:O2'     | 2.25                     | 0.54              |
| 21:U:15:ARG:HB2   | 48:WA:4620:G:H5''  | 1.89                     | 0.54              |
| 22:V:8:PHE:HZ     | 22:V:49:ILE:HD12   | 1.72                     | 0.54              |
| 43:RA:9:GLU:O     | 43:RA:65:GLN:NE2   | 2.40                     | 0.54              |
| 48:WA:261:G:H2'   | 48:WA:262:G:C8     | 2.42                     | 0.54              |
| 48:WA:419:A:N3    | 48:WA:1334:C:O2'   | 2.38                     | 0.54              |
| 48:WA:1247:C:H2'  | 48:WA:1248:G:H8    | 1.72                     | 0.54              |
| 84:GC:67:SER:H    | 84:GC:82:SER:HA    | 1.72                     | 0.54              |
| 6:F:75:ARG:NE     | 48:WA:731:G:OP2    | 2.39                     | 0.54              |
| 13:M:65:ARG:NH2   | 48:WA:2459:G:OP1   | 2.39                     | 0.54              |
| 13:M:68:ARG:HA    | 13:M:98:LEU:HD21   | 1.89                     | 0.54              |
| 48:WA:4718:C:H2'  | 48:WA:4719:A:H8    | 1.70                     | 0.54              |
| 51:ZA:168:C:OP1   | 58:GB:131:ARG:NH1  | 2.40                     | 0.54              |
| 57:FB:140:ASP:OD2 | 80:CC:44:ARG:NH1   | 2.40                     | 0.54              |
| 60:IB:178:ARG:HE  | 60:IB:181:GLN:HG3  | 1.72                     | 0.54              |
| 81:DC:5:GLN:O     | 81:DC:9:SER:OG     | 2.25                     | 0.54              |
| 42:PA:107:ARG:NH2 | 48:WA:2265:A:OP1   | 2.40                     | 0.54              |
| 48:WA:85:G:O2'    | 48:WA:97:G:O6      | 2.25                     | 0.54              |
| 48:WA:3719:A:OP2  | 48:WA:3737:G:N2    | 2.39                     | 0.54              |
| 48:WA:3811:G:N2   | 48:WA:3811:G:OP2   | 2.39                     | 0.54              |
| 48:WA:4240:G:H2'  | 48:WA:4241:A:H8    | 1.72                     | 0.54              |
| 48:WA:4305:C:H2'  | 48:WA:4307:G:H8    | 1.73                     | 0.54              |
| 51:ZA:912:C:H3'   | 51:ZA:913:A:H3'    | 1.89                     | 0.54              |
| 52:AB:85:ARG:HH21 | 52:AB:201:LEU:HD12 | 1.71                     | 0.54              |
| 53:BB:40:ASN:OD1  | 53:BB:75:GLN:NE2   | 2.41                     | 0.54              |
| 58:GB:39:ASP:HB3  | 58:GB:47:GLY:H     | 1.72                     | 0.54              |
| 1:A:225:ILE:HD11  | 1:A:233:ARG:HG3    | 1.90                     | 0.54              |
| 2:B:57:VAL:HG22   | 2:B:73:VAL:HG22    | 1.89                     | 0.54              |
| 16:P:88:ASP:OD2   | 16:P:108:ARG:NH1   | 2.39                     | 0.54              |
| 17:Q:160:GLU:OE1  | 17:Q:163:ARG:NH2   | 2.39                     | 0.54              |
| 23:W:48:ARG:NH2   | 48:WA:2476:G:OP2   | 2.38                     | 0.54              |
| 41:OA:38:THR:HA   | 41:OA:45:THR:HA    | 1.89                     | 0.54              |
| 42:PA:38:PHE:O    | 42:PA:45:HIS:NE2   | 2.32                     | 0.54              |
| 51:ZA:1401:A:H4'  | 72:UB:52:GLY:HA3   | 1.90                     | 0.54              |
| 65:NB:5:HIS:HB3   | 65:NB:117:LEU:HD13 | 1.90                     | 0.54              |
| 79:BC:74:THR:OG1  | 79:BC:77:CYS:SG    | 2.66                     | 0.54              |
| 4:D:124:GLU:OE1   | 4:D:126:THR:OG1    | 2.24                     | 0.54              |
| 16:P:151:HIS:ND1  | 16:P:164:LYS:O     | 2.40                     | 0.54              |
| 48:WA:484:G:H5'   | 48:WA:485:U:H5''   | 1.88                     | 0.54              |
| 49:XA:110:G:H2'   | 49:XA:111:C:C6     | 2.42                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 51:ZA:562:U:H2'   | 51:ZA:563:G:C8    | 2.43                     | 0.54              |
| 51:ZA:948:C:H2'   | 51:ZA:949:G:H8    | 1.73                     | 0.54              |
| 51:ZA:1179:G:N2   | 51:ZA:1182:A:OP2  | 2.40                     | 0.54              |
| 76:YB:102:THR:O   | 76:YB:107:ARG:NH2 | 2.41                     | 0.54              |
| 84:GC:294:ASP:OD2 | 84:GC:296:GLN:NE2 | 2.37                     | 0.54              |
| 3:C:301:ALA:HB1   | 16:P:132:LYS:HE3  | 1.89                     | 0.54              |
| 18:R:127:MET:HA   | 19:S:153:PRO:HD2  | 1.90                     | 0.54              |
| 51:ZA:155:G:H2'   | 51:ZA:156:G:H8    | 1.72                     | 0.54              |
| 51:ZA:571:U:O2'   | 76:YB:60:PHE:O    | 2.25                     | 0.54              |
| 51:ZA:866:U:H2'   | 51:ZA:867:G:C8    | 2.43                     | 0.54              |
| 59:HB:268:LEU:O   | 59:HB:272:SER:HB3 | 2.07                     | 0.54              |
| 2:B:117:ARG:NH2   | 48:WA:4987:U:OP1  | 2.34                     | 0.54              |
| 11:K:178:ALA:N    | 26:Z:134:GLU:OE2  | 2.41                     | 0.54              |
| 46:UA:17:G:H21    | 46:UA:58:A:H5'    | 1.72                     | 0.54              |
| 48:WA:126:C:H2'   | 48:WA:127:G:H8    | 1.71                     | 0.54              |
| 48:WA:2000:A:H2'  | 48:WA:2001:A:C8   | 2.43                     | 0.54              |
| 48:WA:2523:G:H2'  | 48:WA:2524:G:H8   | 1.72                     | 0.54              |
| 51:ZA:626:G:N2    | 51:ZA:626:G:OP2   | 2.41                     | 0.54              |
| 52:AB:77:ILE:HG12 | 52:AB:99:ILE:HB   | 1.89                     | 0.54              |
| 60:IB:4:SER:OG    | 60:IB:6:ASP:OD2   | 2.24                     | 0.54              |
| 4:D:17:GLN:O      | 48:WA:4267:U:N3   | 2.34                     | 0.54              |
| 13:M:184:ILE:O    | 13:M:194:ARG:NH2  | 2.40                     | 0.54              |
| 22:V:80:ARG:HH21  | 58:GB:131:ARG:HG2 | 1.73                     | 0.54              |
| 28:BA:50:ASN:ND2  | 28:BA:75:SER:O    | 2.40                     | 0.54              |
| 48:WA:4763:G:N2   | 48:WA:4768:C:O3'  | 2.41                     | 0.54              |
| 51:ZA:913:A:N6    | 59:HB:357:SER:O   | 2.41                     | 0.54              |
| 56:EB:175:PHE:HE2 | 56:EB:198:ARG:HD2 | 1.72                     | 0.54              |
| 58:GB:55:GLY:H    | 58:GB:63:MET:HE2  | 1.73                     | 0.54              |
| 60:IB:80:ASP:OD1  | 60:IB:81:VAL:N    | 2.40                     | 0.54              |
| 3:C:195:LYS:HE3   | 48:WA:2335:G:H5'' | 1.89                     | 0.54              |
| 30:DA:98:GLU:OE1  | 48:WA:2326:C:O2'  | 2.25                     | 0.54              |
| 48:WA:132:G:O6    | 48:WA:137:G:N1    | 2.41                     | 0.54              |
| 48:WA:1335:A:H2'  | 48:WA:1336:A:H8   | 1.73                     | 0.54              |
| 48:WA:2481:G:H2'  | 48:WA:2482:G:C8   | 2.43                     | 0.54              |
| 51:ZA:1276:A:H1'  | 62:KB:50:GLN:HE22 | 1.72                     | 0.54              |
| 51:ZA:1654:G:OP1  | 71:TB:90:SER:OG   | 2.21                     | 0.54              |
| 56:EB:137:PRO:HB2 | 56:EB:150:PRO:HD2 | 1.90                     | 0.54              |
| 70:SB:20:ILE:HD11 | 70:SB:33:ILE:HG13 | 1.89                     | 0.54              |
| 14:N:65:ASN:ND2   | 48:WA:4567:C:OP1  | 2.34                     | 0.54              |
| 37:KA:5:LYS:NZ    | 48:WA:2409:G:N7   | 2.56                     | 0.54              |
| 48:WA:261:G:H2'   | 48:WA:262:G:H8    | 1.72                     | 0.54              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 48:WA:1727:U:H2'   | 48:WA:1728:U:H6   | 1.73                     | 0.54              |
| 48:WA:1826:G:H2'   | 48:WA:1827:A:H8   | 1.72                     | 0.54              |
| 59:HB:307:LEU:HD22 | 59:HB:334:ALA:HB2 | 1.89                     | 0.54              |
| 59:HB:383:ARG:NH1  | 74:WB:49:GLU:OE2  | 2.40                     | 0.54              |
| 6:F:91:VAL:O       | 6:F:119:GLY:HA2   | 2.08                     | 0.53              |
| 48:WA:2747:A:H2'   | 48:WA:2748:A:H8   | 1.73                     | 0.53              |
| 48:WA:3807:U:H2'   | 48:WA:3808:G:H8   | 1.73                     | 0.53              |
| 48:WA:4239:C:O2'   | 48:WA:4323:U:O2   | 2.26                     | 0.53              |
| 78:AC:59:PHE:HB2   | 78:AC:62:TYR:HB2  | 1.90                     | 0.53              |
| 2:B:254:ILE:HG21   | 2:B:262:VAL:HG22  | 1.90                     | 0.53              |
| 18:R:174:THR:OG1   | 48:WA:4765:U:O2'  | 2.23                     | 0.53              |
| 46:UA:30:G:N7      | 46:UA:41:G:N2     | 2.55                     | 0.53              |
| 47:VA:21:C:OP1     | 51:ZA:1704:C:N4   | 2.42                     | 0.53              |
| 48:WA:1505:A:H4'   | 48:WA:1506:G:H5'  | 1.90                     | 0.53              |
| 48:WA:3725:A:H2'   | 48:WA:3726:A:H8   | 1.73                     | 0.53              |
| 51:ZA:981:A:H2'    | 51:ZA:982:G:C8    | 2.44                     | 0.53              |
| 58:GB:165:GLU:OE1  | 58:GB:167:LYS:NZ  | 2.39                     | 0.53              |
| 84:GC:255:SER:OG   | 84:GC:257:LYS:NZ  | 2.41                     | 0.53              |
| 5:E:48:ARG:O       | 5:E:67:ARG:NH1    | 2.42                     | 0.53              |
| 17:Q:60:ARG:HH12   | 48:WA:2617:C:H5'' | 1.73                     | 0.53              |
| 37:KA:23:ILE:HG23  | 37:KA:38:ASN:HB2  | 1.90                     | 0.53              |
| 51:ZA:111:A:O2'    | 63:LB:69:ARG:NH1  | 2.42                     | 0.53              |
| 51:ZA:547:G:H2'    | 51:ZA:549:C:H6    | 1.74                     | 0.53              |
| 51:ZA:844:U:OP1    | 56:EB:240:ARG:NH1 | 2.42                     | 0.53              |
| 51:ZA:1293:A:N6    | 51:ZA:1294:G:O6   | 2.41                     | 0.53              |
| 57:FB:124:ASP:OD2  | 80:CC:47:LYS:NZ   | 2.40                     | 0.53              |
| 76:YB:13:MET:SD    | 76:YB:22:GLN:NE2  | 2.79                     | 0.53              |
| 17:Q:44:LEU:HD22   | 17:Q:49:LEU:HD12  | 1.90                     | 0.53              |
| 18:R:95:ARG:NH2    | 48:WA:1953:G:O2'  | 2.41                     | 0.53              |
| 48:WA:1074:G:N2    | 48:WA:1075:G:O6   | 2.41                     | 0.53              |
| 48:WA:2460:C:O2    | 48:WA:3673:G:N2   | 2.41                     | 0.53              |
| 48:WA:4962:G:H2'   | 48:WA:4963:G:H8   | 1.73                     | 0.53              |
| 51:ZA:375:U:OP2    | 63:LB:59:LYS:NZ   | 2.41                     | 0.53              |
| 51:ZA:1711:U:H2'   | 51:ZA:1712:A:C8   | 2.43                     | 0.53              |
| 79:BC:54:VAL:HG13  | 79:BC:63:LEU:HB2  | 1.90                     | 0.53              |
| 9:I:118:ALA:O      | 48:WA:1866:G:O2'  | 2.23                     | 0.53              |
| 14:N:12:ARG:O      | 18:R:171:ARG:NH2  | 2.39                     | 0.53              |
| 15:O:164:ARG:NH2   | 48:WA:1598:U:O2'  | 2.41                     | 0.53              |
| 18:R:132:ILE:HG23  | 18:R:136:LYS:HB2  | 1.91                     | 0.53              |
| 48:WA:2000:A:N3    | 48:WA:2021:C:O2'  | 2.40                     | 0.53              |
| 48:WA:2380:G:N2    | 48:WA:2383:A:OP2  | 2.39                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 48:WA:4763:G:H2'   | 48:WA:4764:A:H8    | 1.72                     | 0.53              |
| 2:B:261:ARG:HB2    | 14:N:64:THR:HG21   | 1.90                     | 0.53              |
| 5:E:275:ARG:NH2    | 48:WA:4886:G:N7    | 2.57                     | 0.53              |
| 14:N:188:LYS:NZ    | 48:WA:4895:A:OP1   | 2.42                     | 0.53              |
| 48:WA:4969:A:H2'   | 48:WA:4970:A:H8    | 1.74                     | 0.53              |
| 51:ZA:980:A:H2'    | 51:ZA:981:A:C8     | 2.44                     | 0.53              |
| 56:EB:252:ARG:NH1  | 61:JB:75:ASN:OD1   | 2.42                     | 0.53              |
| 2:B:189:THR:HG23   | 2:B:192:GLU:H      | 1.73                     | 0.53              |
| 3:C:323:ARG:HB2    | 48:WA:1283:G:H5'   | 1.91                     | 0.53              |
| 7:G:126:ARG:NH2    | 48:WA:4164:C:O2    | 2.35                     | 0.53              |
| 48:WA:2460:C:O2'   | 48:WA:3673:G:N3    | 2.39                     | 0.53              |
| 48:WA:3666:G:H2'   | 48:WA:3667:G:H8    | 1.74                     | 0.53              |
| 48:WA:4241:A:H2'   | 48:WA:4242:G:C8    | 2.44                     | 0.53              |
| 50:YA:64:U:H2'     | 50:YA:65:A:H8      | 1.73                     | 0.53              |
| 51:ZA:1864:U:H5'   | 78:AC:79:ILE:HD11  | 1.90                     | 0.53              |
| 87:c:241:SER:HB3   | 87:c:244:SER:HB3   | 1.89                     | 0.53              |
| 6:F:121:PHE:O      | 6:F:204:ASN:ND2    | 2.41                     | 0.53              |
| 34:HA:29:ARG:HH22  | 48:WA:276:C:H2'    | 1.73                     | 0.53              |
| 40:NA:8:ARG:NH2    | 48:WA:4234:U:O4    | 2.38                     | 0.53              |
| 48:WA:115:C:O2'    | 48:WA:276:C:OP1    | 2.26                     | 0.53              |
| 48:WA:425:U:H2'    | 48:WA:426:A:H8     | 1.73                     | 0.53              |
| 48:WA:2297:C:H2'   | 48:WA:2298:G:H8    | 1.73                     | 0.53              |
| 48:WA:4770:G:H2'   | 48:WA:4771:G:H8    | 1.74                     | 0.53              |
| 51:ZA:172:U:N3     | 51:ZA:337:C:O2'    | 2.41                     | 0.53              |
| 51:ZA:1086:G:OP2   | 78:AC:12:LYS:NZ    | 2.37                     | 0.53              |
| 51:ZA:1215:C:O2'   | 51:ZA:1645:C:OP2   | 2.26                     | 0.53              |
| 56:EB:251:GLU:OE2  | 56:EB:255:ARG:NH2  | 2.41                     | 0.53              |
| 84:GC:166:VAL:HG22 | 84:GC:176:VAL:HG22 | 1.90                     | 0.53              |
| 84:GC:257:LYS:HG2  | 84:GC:269:GLU:HG3  | 1.89                     | 0.53              |
| 5:E:52:LEU:HG      | 5:E:53:VAL:HG23    | 1.90                     | 0.53              |
| 7:G:156:ARG:NH2    | 7:G:245:ARG:O      | 2.42                     | 0.53              |
| 48:WA:417:G:OP1    | 48:WA:2331:U:O2'   | 2.25                     | 0.53              |
| 48:WA:1183:U:H2'   | 48:WA:1184:G:C8    | 2.44                     | 0.53              |
| 48:WA:1565:A:H2'   | 48:WA:1566:A:C8    | 2.44                     | 0.53              |
| 51:ZA:107:A:H2'    | 51:ZA:108:G:C8     | 2.44                     | 0.53              |
| 51:ZA:642:U:H4'    | 51:ZA:644:G:H4'    | 1.91                     | 0.53              |
| 51:ZA:1418:C:OP2   | 51:ZA:1420:G:N2    | 2.41                     | 0.53              |
| 51:ZA:1598:G:OP1   | 77:ZB:80:ARG:NH1   | 2.42                     | 0.53              |
| 2:B:77:THR:HG21    | 2:B:337:VAL:HG22   | 1.90                     | 0.53              |
| 3:C:312:ARG:NH2    | 48:WA:2077:G:OP1   | 2.41                     | 0.53              |
| 13:M:155:VAL:O     | 13:M:162:ARG:NH2   | 2.42                     | 0.53              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 19:S:46:GLY:O     | 19:S:49:GLN:NE2    | 2.42                     | 0.53              |
| 48:WA:417:G:H1'   | 50:YA:17:A:H61     | 1.74                     | 0.53              |
| 51:ZA:1808:U:H2'  | 51:ZA:1809:A:C8    | 2.44                     | 0.53              |
| 84:GC:77:PHE:HB3  | 84:GC:89:LEU:HD11  | 1.91                     | 0.53              |
| 84:GC:237:ASN:ND2 | 84:GC:286:CYS:O    | 2.38                     | 0.53              |
| 6:F:95:ARG:NH2    | 48:WA:1897:G:OP1   | 2.41                     | 0.52              |
| 48:WA:246:G:H2'   | 48:WA:247:G:H8     | 1.73                     | 0.52              |
| 48:WA:4994:G:H2'  | 48:WA:4995:G:C8    | 2.43                     | 0.52              |
| 51:ZA:1203:G:H2'  | 51:ZA:1204:A:C8    | 2.44                     | 0.52              |
| 51:ZA:1623:A:H5'' | 70:SB:133:GLY:HA3  | 1.91                     | 0.52              |
| 56:EB:199:GLU:HB3 | 56:EB:207:VAL:HG13 | 1.89                     | 0.52              |
| 86:b:35:VAL:HG23  | 86:b:40:MET:HG2    | 1.91                     | 0.52              |
| 20:T:63:LEU:HG    | 20:T:72:VAL:HG22   | 1.90                     | 0.52              |
| 40:NA:80:LYS:O    | 48:WA:4348:U:O2'   | 2.25                     | 0.52              |
| 48:WA:2871:U:O2'  | 48:WA:2883:A:N7    | 2.35                     | 0.52              |
| 51:ZA:183:G:O2'   | 51:ZA:184:G:O5'    | 2.26                     | 0.52              |
| 51:ZA:847:A:OP1   | 56:EB:108:ARG:NH2  | 2.42                     | 0.52              |
| 51:ZA:941:C:H2'   | 51:ZA:942:G:C8     | 2.44                     | 0.52              |
| 54:CB:244:ILE:O   | 54:CB:247:THR:OG1  | 2.25                     | 0.52              |
| 88:HC:241:PRO:HB3 | 88:HC:244:LYS:HD2  | 1.90                     | 0.52              |
| 42:PA:90:LEU:HG   | 42:PA:111:ILE:HG23 | 1.91                     | 0.52              |
| 51:ZA:1428:G:O6   | 68:QB:99:LYS:NZ    | 2.42                     | 0.52              |
| 51:ZA:1781:A:H2'  | 51:ZA:1782:G:C8    | 2.44                     | 0.52              |
| 86:b:69:LEU:HD21  | 86:b:76:GLU:HB2    | 1.90                     | 0.52              |
| 7:G:194:ASN:ND2   | 48:WA:151:G:N7     | 2.57                     | 0.52              |
| 13:M:49:ARG:HH12  | 48:WA:152:U:P      | 2.32                     | 0.52              |
| 16:P:172:ARG:HD2  | 26:Z:57:GLY:HA3    | 1.92                     | 0.52              |
| 17:Q:97:ARG:NH2   | 48:WA:2727:A:OP2   | 2.43                     | 0.52              |
| 23:W:110:LYS:NZ   | 23:W:121:VAL:O     | 2.42                     | 0.52              |
| 30:DA:29:VAL:HB   | 48:WA:1334:C:H5''  | 1.91                     | 0.52              |
| 48:WA:3909:G:N2   | 85:IC:197:PHE:O    | 2.41                     | 0.52              |
| 48:WA:4706:C:H2'  | 48:WA:4707:A:H8    | 1.75                     | 0.52              |
| 64:MB:47:ALA:HA   | 64:MB:112:LYS:HB3  | 1.91                     | 0.52              |
| 2:B:95:THR:HG22   | 48:WA:4912:A:H4'   | 1.92                     | 0.52              |
| 10:J:112:HIS:HE1  | 10:J:125:ILE:HA    | 1.74                     | 0.52              |
| 25:Y:51:ARG:HB2   | 25:Y:65:ARG:HE     | 1.75                     | 0.52              |
| 29:CA:70:LYS:HE2  | 48:WA:2391:A:H5'   | 1.92                     | 0.52              |
| 33:GA:89:ARG:NH1  | 50:YA:37:A:OP2     | 2.41                     | 0.52              |
| 48:WA:2413:C:O2'  | 48:WA:2528:C:O2    | 2.23                     | 0.52              |
| 68:QB:45:ALA:HB2  | 68:QB:101:GLY:HA3  | 1.92                     | 0.52              |
| 74:WB:66:THR:HG21 | 74:WB:68:ARG:HH11  | 1.75                     | 0.52              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:B:223:THR:HB    | 2:B:275:HIS:H    | 1.75                     | 0.52              |
| 2:B:324:GLY:HA2   | 48:WA:5053:C:H4' | 1.91                     | 0.52              |
| 3:C:4:ALA:O       | 3:C:29:LYS:NZ    | 2.40                     | 0.52              |
| 11:K:79:GLU:OE1   | 11:K:82:ARG:NH1  | 2.42                     | 0.52              |
| 17:Q:39:GLN:NE2   | 48:WA:2713:G:OP2 | 2.42                     | 0.52              |
| 21:U:21:PRO:HA    | 21:U:54:ALA:HA   | 1.90                     | 0.52              |
| 29:CA:24:GLU:OE2  | 29:CA:87:ARG:NH1 | 2.42                     | 0.52              |
| 48:WA:2523:G:H2'  | 48:WA:2524:G:C8  | 2.44                     | 0.52              |
| 48:WA:3724:G:H2'  | 48:WA:3725:A:H8  | 1.73                     | 0.52              |
| 48:WA:3918:G:H2'  | 48:WA:3919:A:H8  | 1.75                     | 0.52              |
| 51:ZA:145:G:H2'   | 51:ZA:146:G:C8   | 2.44                     | 0.52              |
| 51:ZA:1245:G:N2   | 72:UB:72:GLU:OE2 | 2.42                     | 0.52              |
| 2:B:13:SER:HB2    | 48:WA:4624:A:H4' | 1.92                     | 0.52              |
| 6:F:241:ARG:NH2   | 48:WA:945:C:OP1  | 2.39                     | 0.52              |
| 10:J:32:ARG:HD2   | 10:J:35:ARG:HH22 | 1.75                     | 0.52              |
| 11:K:87:HIS:HB3   | 11:K:90:VAL:HG23 | 1.92                     | 0.52              |
| 17:Q:88:ARG:O     | 48:WA:2727:A:N6  | 2.43                     | 0.52              |
| 20:T:105:ASN:HD21 | 20:T:111:GLU:HB2 | 1.74                     | 0.52              |
| 25:Y:17:ARG:NH2   | 25:Y:18:TYR:OH   | 2.42                     | 0.52              |
| 40:NA:26:TYR:HB3  | 40:NA:67:VAL:HB  | 1.92                     | 0.52              |
| 48:WA:436:C:H2'   | 48:WA:437:G:H8   | 1.75                     | 0.52              |
| 48:WA:2742:U:O2'  | 48:WA:2744:G:N2  | 2.43                     | 0.52              |
| 62:KB:20:VAL:HG23 | 62:KB:70:TYR:HA  | 1.92                     | 0.52              |
| 86:b:28:PHE:HB2   | 86:b:89:VAL:HG22 | 1.91                     | 0.52              |
| 17:Q:62:ARG:NH1   | 48:WA:4647:C:OP2 | 2.42                     | 0.52              |
| 25:Y:52:LYS:O     | 25:Y:65:ARG:NH2  | 2.43                     | 0.52              |
| 48:WA:1776:C:H2'  | 48:WA:1777:A:H8  | 1.74                     | 0.52              |
| 48:WA:1897:G:O2'  | 48:WA:1909:A:N3  | 2.37                     | 0.52              |
| 48:WA:4095:G:H22  | 48:WA:4117:G:H1  | 1.58                     | 0.52              |
| 51:ZA:1288:U:H3   | 51:ZA:1311:C:N4  | 1.99                     | 0.52              |
| 51:ZA:1630:A:H5'' | 70:SB:37:GLY:N   | 2.24                     | 0.52              |
| 3:C:343:GLN:HG2   | 48:WA:725:C:H1'  | 1.92                     | 0.52              |
| 35:IA:27:TYR:HA   | 35:IA:34:CYS:HA  | 1.90                     | 0.52              |
| 43:RA:61:LYS:HB2  | 43:RA:72:GLU:HG2 | 1.92                     | 0.52              |
| 48:WA:2469:U:H4'  | 48:WA:2470:U:H5' | 1.92                     | 0.52              |
| 48:WA:3612:A:H2'  | 48:WA:3613:A:H8  | 1.74                     | 0.52              |
| 48:WA:3691:G:O2'  | 48:WA:3820:U:OP2 | 2.26                     | 0.52              |
| 48:WA:4232:C:H1'  | 48:WA:4273:A:N1  | 2.25                     | 0.52              |
| 50:YA:71:A:H4'    | 50:YA:72:A:H5'   | 1.92                     | 0.52              |
| 51:ZA:1016:U:H5'' | 65:NB:14:SER:HB2 | 1.91                     | 0.52              |
| 51:ZA:1617:G:O6   | 67:PB:43:ARG:NH1 | 2.42                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 51:ZA:1630:A:H5''  | 70:SB:37:GLY:H     | 1.75                     | 0.52              |
| 72:UB:46:LYS:NZ    | 72:UB:97:ILE:O     | 2.42                     | 0.52              |
| 12:L:39:ASP:HB2    | 12:L:47:ARG:HE     | 1.75                     | 0.52              |
| 31:EA:43:LEU:HB2   | 31:EA:109:ARG:HH12 | 1.75                     | 0.52              |
| 48:WA:1249:U:O2    | 48:WA:1268:G:N2    | 2.36                     | 0.52              |
| 48:WA:1384:G:H2'   | 48:WA:1385:G:H8    | 1.74                     | 0.52              |
| 51:ZA:432:G:H2'    | 51:ZA:433:A:C8     | 2.44                     | 0.52              |
| 51:ZA:521:A:OP1    | 61:JB:45:ARG:NH1   | 2.38                     | 0.52              |
| 51:ZA:639:C:H2'    | 51:ZA:640:A:C8     | 2.46                     | 0.52              |
| 86:b:116:ILE:HG22  | 86:b:118:PRO:HD2   | 1.91                     | 0.52              |
| 1:A:30:ARG:O       | 1:A:163:ARG:NH2    | 2.42                     | 0.51              |
| 18:R:15:ARG:HH21   | 19:S:141:VAL:HG22  | 1.75                     | 0.51              |
| 21:U:43:LYS:HD2    | 48:WA:4510:C:H5''  | 1.92                     | 0.51              |
| 26:Z:75:LEU:HG     | 26:Z:113:GLY:HA2   | 1.92                     | 0.51              |
| 42:PA:31:ASN:ND2   | 42:PA:40:TYR:O     | 2.43                     | 0.51              |
| 48:WA:1210:C:H2'   | 48:WA:1211:G:H8    | 1.74                     | 0.51              |
| 48:WA:1335:A:H2'   | 48:WA:1336:A:C8    | 2.45                     | 0.51              |
| 48:WA:1657:C:O2    | 48:WA:4392:A:O2'   | 2.28                     | 0.51              |
| 51:ZA:432:G:H2'    | 51:ZA:433:A:H8     | 1.75                     | 0.51              |
| 51:ZA:1692:U:H2'   | 51:ZA:1693:G:C8    | 2.45                     | 0.51              |
| 57:FB:71:ARG:NH2   | 57:FB:148:ASN:OD1  | 2.33                     | 0.51              |
| 66:OB:93:LEU:HD23  | 66:OB:119:LEU:HD13 | 1.92                     | 0.51              |
| 2:B:254:ILE:HG23   | 2:B:266:VAL:HG11   | 1.93                     | 0.51              |
| 10:J:44:THR:O      | 10:J:78:LYS:NZ     | 2.36                     | 0.51              |
| 14:N:163:LYS:NZ    | 48:WA:4911:A:OP1   | 2.42                     | 0.51              |
| 40:NA:64:LYS:HD2   | 48:WA:4372:G:H5''  | 1.91                     | 0.51              |
| 51:ZA:1004:U:H2'   | 51:ZA:1005:G:C8    | 2.45                     | 0.51              |
| 55:DB:144:ARG:HG3  | 55:DB:213:VAL:HG22 | 1.93                     | 0.51              |
| 56:EB:127:ARG:N    | 56:EB:140:VAL:O    | 2.34                     | 0.51              |
| 56:EB:128:LYS:HG2  | 56:EB:140:VAL:HB   | 1.92                     | 0.51              |
| 20:T:44:GLN:HA     | 20:T:56:LEU:HD21   | 1.92                     | 0.51              |
| 48:WA:1507:C:H2'   | 48:WA:1508:G:H8    | 1.76                     | 0.51              |
| 48:WA:1997:G:O2'   | 86:b:48:ARG:NH1    | 2.43                     | 0.51              |
| 48:WA:2445:G:OP2   | 48:WA:2518:G:N2    | 2.37                     | 0.51              |
| 51:ZA:56:G:OP1     | 76:YB:111:LYS:NZ   | 2.42                     | 0.51              |
| 60:IB:27:TYR:HB3   | 60:IB:49:ARG:HH12  | 1.75                     | 0.51              |
| 60:IB:64:ASN:O     | 60:IB:186:ASP:HA   | 2.10                     | 0.51              |
| 60:IB:162:LEU:HD11 | 60:IB:191:GLU:HG2  | 1.91                     | 0.51              |
| 70:SB:24:ARG:HH21  | 70:SB:28:PHE:HB3   | 1.75                     | 0.51              |
| 5:E:144:ARG:NH2    | 5:E:194:GLN:O      | 2.44                     | 0.51              |
| 13:M:35:ALA:HA     | 13:M:65:ARG:HG2    | 1.93                     | 0.51              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 24:X:11:ARG:HG3   | 48:WA:229:G:H5''   | 1.91                     | 0.51              |
| 40:NA:4:VAL:O     | 40:NA:94:GLY:N     | 2.39                     | 0.51              |
| 42:PA:103:HIS:ND1 | 42:PA:105:ASP:OD1  | 2.40                     | 0.51              |
| 48:WA:3882:G:H2'  | 48:WA:3883:G:C8    | 2.45                     | 0.51              |
| 51:ZA:17:C:H2'    | 51:ZA:18:C:C6      | 2.46                     | 0.51              |
| 56:EB:44:LEU:HD21 | 56:EB:70:ILE:HG21  | 1.93                     | 0.51              |
| 3:C:306:ARG:HG2   | 48:WA:2101:C:H3'   | 1.92                     | 0.51              |
| 13:M:9:GLU:HB2    | 34:HA:44:ILE:HG13  | 1.93                     | 0.51              |
| 13:M:138:PHE:HA   | 13:M:143:ARG:HH21  | 1.76                     | 0.51              |
| 19:S:83:LYS:NZ    | 48:WA:4307:G:O5'   | 2.43                     | 0.51              |
| 48:WA:1343:U:H2'  | 48:WA:1344:A:H8    | 1.75                     | 0.51              |
| 48:WA:1734:C:H2'  | 48:WA:1735:G:C8    | 2.46                     | 0.51              |
| 48:WA:2519:A:N3   | 48:WA:2541:C:O2'   | 2.43                     | 0.51              |
| 48:WA:2892:C:H42  | 48:WA:3613:A:H61   | 1.59                     | 0.51              |
| 48:WA:3734:A:H2'  | 48:WA:3735:A:C8    | 2.45                     | 0.51              |
| 48:WA:3872:C:H2'  | 48:WA:3873:A:H8    | 1.76                     | 0.51              |
| 51:ZA:317:C:OP2   | 58:GB:183:ARG:NH2  | 2.42                     | 0.51              |
| 84:GC:223:GLU:HB2 | 84:GC:225:LYS:HE3  | 1.91                     | 0.51              |
| 8:H:155:SER:OG    | 48:WA:4690:C:O2'   | 2.28                     | 0.51              |
| 13:M:73:ARG:NH1   | 48:WA:32:G:OP1     | 2.44                     | 0.51              |
| 35:IA:19:CYS:HB3  | 35:IA:22:CYS:SG    | 2.50                     | 0.51              |
| 45:TA:22:G:H2'    | 45:TA:23:A:H8      | 1.75                     | 0.51              |
| 48:WA:1264:G:H2'  | 48:WA:1265:A:C8    | 2.46                     | 0.51              |
| 48:WA:1373:A:N1   | 50:YA:28:C:O2'     | 2.40                     | 0.51              |
| 48:WA:2761:G:O2'  | 48:WA:2762:G:O4'   | 2.25                     | 0.51              |
| 48:WA:3920:G:OP2  | 93:WA:5229:SPD:N10 | 2.42                     | 0.51              |
| 51:ZA:110:U:H3    | 51:ZA:351:G:H1     | 1.59                     | 0.51              |
| 51:ZA:583:A:H3'   | 51:ZA:584:A:H8     | 1.75                     | 0.51              |
| 51:ZA:640:A:H2'   | 51:ZA:641:A:C8     | 2.45                     | 0.51              |
| 51:ZA:1375:G:H2'  | 51:ZA:1376:A:C8    | 2.45                     | 0.51              |
| 52:AB:158:ASP:OD1 | 73:VB:60:ARG:NH1   | 2.39                     | 0.51              |
| 79:BC:42:LYS:NZ   | 79:BC:43:ILE:O     | 2.44                     | 0.51              |
| 84:GC:45:LEU:HB3  | 84:GC:47:ARG:HD3   | 1.92                     | 0.51              |
| 84:GC:132:TRP:CD1 | 84:GC:138:CYS:HA   | 2.46                     | 0.51              |
| 25:Y:92:ASP:OD2   | 25:Y:94:THR:OG1    | 2.21                     | 0.51              |
| 48:WA:1525:A:N3   | 48:WA:4391:C:O2'   | 2.42                     | 0.51              |
| 48:WA:1944:A:H2'  | 48:WA:1945:A:C8    | 2.46                     | 0.51              |
| 48:WA:2416:G:H2'  | 48:WA:2417:U:H6    | 1.75                     | 0.51              |
| 48:WA:2485:G:H2'  | 48:WA:2486:A:H8    | 1.76                     | 0.51              |
| 48:WA:4577:G:N3   | 48:WA:5070:G:O2'   | 2.43                     | 0.51              |
| 48:WA:4969:A:H2'  | 48:WA:4970:A:C8    | 2.45                     | 0.51              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 51:ZA:520:A:O2'   | 51:ZA:825:A:N3     | 2.36                     | 0.51              |
| 79:BC:67:THR:OG1  | 79:BC:70:LYS:O     | 2.28                     | 0.51              |
| 3:C:328:LEU:HD13  | 6:F:186:MET:HE2    | 1.93                     | 0.51              |
| 37:KA:24:PRO:HG2  | 37:KA:27:ILE:HB    | 1.93                     | 0.51              |
| 48:WA:1507:C:H2'  | 48:WA:1508:G:C8    | 2.46                     | 0.51              |
| 48:WA:2467:C:H1'  | 48:WA:3674:G:H1    | 1.75                     | 0.51              |
| 48:WA:2498:G:H2'  | 48:WA:2499:C:C6    | 2.45                     | 0.51              |
| 48:WA:4090:C:H2'  | 48:WA:4091:G:C8    | 2.46                     | 0.51              |
| 51:ZA:1670:C:H2'  | 51:ZA:1671:G:H8    | 1.76                     | 0.51              |
| 54:CB:65:LYS:HG3  | 54:CB:273:LEU:HD22 | 1.93                     | 0.51              |
| 88:HC:249:PRO:HB3 | 88:HC:364:HIS:HB2  | 1.92                     | 0.51              |
| 2:B:15:GLY:O      | 48:WA:4589:G:N2    | 2.34                     | 0.51              |
| 6:F:136:GLU:OE1   | 49:XA:96:U:O2'     | 2.24                     | 0.51              |
| 12:L:128:LYS:NZ   | 48:WA:4899:G:OP1   | 2.43                     | 0.51              |
| 42:PA:19:LYS:HB2  | 48:WA:2339:C:H4'   | 1.93                     | 0.51              |
| 51:ZA:143:U:H4'   | 51:ZA:144:U:H5'    | 1.93                     | 0.51              |
| 51:ZA:311:C:H5''  | 51:ZA:312:G:H5''   | 1.93                     | 0.51              |
| 51:ZA:436:G:OP2   | 51:ZA:471:G:O2'    | 2.28                     | 0.51              |
| 51:ZA:1758:G:H2'  | 51:ZA:1759:G:H8    | 1.74                     | 0.51              |
| 52:AB:51:LEU:HD23 | 69:RB:105:MET:HE1  | 1.92                     | 0.51              |
| 66:OB:117:ARG:NE  | 78:AC:52:ASP:OD2   | 2.44                     | 0.51              |
| 68:QB:35:SER:OG   | 68:QB:50:HIS:NE2   | 2.41                     | 0.51              |
| 70:SB:36:VAL:HG21 | 70:SB:71:MET:HE3   | 1.92                     | 0.51              |
| 1:A:152:SER:OG    | 48:WA:3663:G:N7    | 2.41                     | 0.51              |
| 12:L:121:ARG:NH2  | 48:WA:4883:U:OP1   | 2.38                     | 0.51              |
| 14:N:55:LEU:HD23  | 14:N:58:LEU:HD12   | 1.93                     | 0.51              |
| 17:Q:90:PRO:HG2   | 17:Q:93:VAL:HB     | 1.93                     | 0.51              |
| 51:ZA:1220:A:N3   | 51:ZA:1677:U:O2'   | 2.37                     | 0.51              |
| 77:ZB:58:LEU:HD12 | 77:ZB:62:VAL:HG21  | 1.93                     | 0.51              |
| 17:Q:59:SER:HA    | 48:WA:2636:C:H5'   | 1.92                     | 0.50              |
| 19:S:91:VAL:HB    | 19:S:96:ILE:HD11   | 1.93                     | 0.50              |
| 45:TA:42:G:H2'    | 45:TA:43:A:H8      | 1.76                     | 0.50              |
| 48:WA:1565:A:N6   | 51:ZA:1028:A:N1    | 2.58                     | 0.50              |
| 48:WA:4637:A:H8   | 48:WA:5050:A:H61   | 1.60                     | 0.50              |
| 48:WA:5059:C:H2'  | 48:WA:5060:A:C8    | 2.46                     | 0.50              |
| 51:ZA:554:A:H1'   | 51:ZA:555:A:H2'    | 1.92                     | 0.50              |
| 54:CB:187:ARG:HE  | 54:CB:192:LEU:HD12 | 1.75                     | 0.50              |
| 55:DB:210:VAL:O   | 55:DB:211:ARG:NH1  | 2.40                     | 0.50              |
| 3:C:35:ASP:OD1    | 3:C:35:ASP:N       | 2.44                     | 0.50              |
| 17:Q:121:HIS:ND1  | 48:WA:2666:G:OP2   | 2.44                     | 0.50              |
| 27:AA:49:HIS:NE2  | 48:WA:1817:G:O6    | 2.39                     | 0.50              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 48:WA:418:A:H4'   | 48:WA:2313:C:H5'   | 1.93                     | 0.50              |
| 48:WA:456:C:H2'   | 48:WA:457:G:C8     | 2.46                     | 0.50              |
| 48:WA:1998:C:H5'  | 86:b:48:ARG:HH11   | 1.75                     | 0.50              |
| 50:YA:84:A:H1'    | 50:YA:85:U:H4'     | 1.93                     | 0.50              |
| 53:BB:144:LYS:HE2 | 53:BB:206:PRO:HB2  | 1.93                     | 0.50              |
| 55:DB:114:ARG:HB2 | 62:KB:22:VAL:HG11  | 1.94                     | 0.50              |
| 61:JB:83:ARG:HD3  | 61:JB:150:ARG:HD3  | 1.92                     | 0.50              |
| 6:F:135:VAL:HG23  | 6:F:139:ILE:HD13   | 1.92                     | 0.50              |
| 9:I:95:HIS:HB3    | 9:I:126:VAL:HG12   | 1.92                     | 0.50              |
| 10:J:29:SER:OG    | 10:J:67:LYS:O      | 2.26                     | 0.50              |
| 27:AA:11:ASN:ND2  | 48:WA:1671:A:OP1   | 2.44                     | 0.50              |
| 46:UA:64:G:OP2    | 46:UA:64:G:N2      | 2.34                     | 0.50              |
| 48:WA:1413:C:N4   | 48:WA:1414:G:O6    | 2.44                     | 0.50              |
| 51:ZA:84:A:N3     | 51:ZA:150:A:O2'    | 2.43                     | 0.50              |
| 51:ZA:155:G:H2'   | 51:ZA:156:G:C8     | 2.47                     | 0.50              |
| 57:FB:59:LYS:HB2  | 57:FB:62:ARG:HB2   | 1.94                     | 0.50              |
| 10:J:84:GLU:OE2   | 10:J:92:TYR:OH     | 2.28                     | 0.50              |
| 28:BA:17:ARG:HD2  | 28:BA:104:ILE:HA   | 1.93                     | 0.50              |
| 51:ZA:5:U:H2'     | 51:ZA:6:G:H8       | 1.76                     | 0.50              |
| 51:ZA:1362:U:H5'' | 51:ZA:1363:C:H5    | 1.76                     | 0.50              |
| 76:YB:20:ARG:NH2  | 76:YB:22:GLN:OE1   | 2.44                     | 0.50              |
| 1:A:132:ASN:ND2   | 48:WA:3685:C:OP1   | 2.43                     | 0.50              |
| 1:A:247:ARG:HB3   | 51:ZA:1069:U:H4'   | 1.94                     | 0.50              |
| 2:B:79:VAL:HB     | 2:B:331:VAL:HG23   | 1.93                     | 0.50              |
| 44:SA:51:C:H2'    | 44:SA:52:G:H8      | 1.77                     | 0.50              |
| 48:WA:1317:C:N4   | 48:WA:1318:G:O6    | 2.44                     | 0.50              |
| 48:WA:1560:A:H2'  | 48:WA:1561:G:C8    | 2.47                     | 0.50              |
| 48:WA:3850:U:H2'  | 48:WA:3851:A:C8    | 2.46                     | 0.50              |
| 48:WA:4080:C:O2'  | 48:WA:4174:A:N6    | 2.44                     | 0.50              |
| 51:ZA:1146:C:O2'  | 51:ZA:1150:A:N1    | 2.42                     | 0.50              |
| 51:ZA:1541:G:H4'  | 71:TB:15:VAL:HG11  | 1.93                     | 0.50              |
| 51:ZA:1711:U:H2'  | 51:ZA:1712:A:H8    | 1.77                     | 0.50              |
| 48:WA:4323:U:H2'  | 48:WA:4324:G:C8    | 2.47                     | 0.50              |
| 51:ZA:553:U:O2'   | 51:ZA:554:A:O5'    | 2.26                     | 0.50              |
| 51:ZA:1018:U:O2'  | 65:NB:86:GLU:OE2   | 2.29                     | 0.50              |
| 51:ZA:1048:G:H21  | 51:ZA:1070:A:H62   | 1.58                     | 0.50              |
| 51:ZA:1245:G:O2'  | 51:ZA:1492:U:OP1   | 2.30                     | 0.50              |
| 51:ZA:1332:A:O2'  | 55:DB:183:GLN:O    | 2.30                     | 0.50              |
| 63:LB:59:LYS:HD3  | 63:LB:134:LEU:HB3  | 1.94                     | 0.50              |
| 88:HC:279:THR:HB  | 88:HC:286:THR:HG23 | 1.92                     | 0.50              |
| 12:L:59:ASP:OD1   | 12:L:59:ASP:N      | 2.45                     | 0.50              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 13:M:172:ARG:NH1  | 48:WA:62:A:OP1     | 2.44                     | 0.50              |
| 33:GA:27:GLU:OE2  | 33:GA:46:LYS:NZ    | 2.42                     | 0.50              |
| 36:JA:12:LEU:HD21 | 36:JA:16:ARG:HH21  | 1.76                     | 0.50              |
| 48:WA:4240:G:H2'  | 48:WA:4241:A:C8    | 2.45                     | 0.50              |
| 48:WA:4406:U:O2'  | 48:WA:4408:U:O4    | 2.29                     | 0.50              |
| 51:ZA:1406:G:H2'  | 51:ZA:1407:U:C6    | 2.47                     | 0.50              |
| 79:BC:23:ARG:NH2  | 79:BC:29:ASN:OD1   | 2.43                     | 0.50              |
| 10:J:27:GLY:HA2   | 10:J:68:ILE:HG23   | 1.93                     | 0.50              |
| 26:Z:103:VAL:HG12 | 26:Z:108:TYR:HB2   | 1.93                     | 0.50              |
| 32:FA:66:ARG:NH2  | 48:WA:2519:A:O2'   | 2.44                     | 0.50              |
| 48:WA:1593:U:H3   | 48:WA:4557:U:H5''  | 1.77                     | 0.50              |
| 48:WA:1944:A:OP2  | 48:WA:2042:A:N6    | 2.39                     | 0.50              |
| 61:JB:59:GLU:O    | 61:JB:62:THR:OG1   | 2.30                     | 0.50              |
| 3:C:56:GLU:OE1    | 3:C:106:LYS:NZ     | 2.44                     | 0.50              |
| 48:WA:3612:A:H2'  | 48:WA:3613:A:C8    | 2.47                     | 0.50              |
| 48:WA:3756:G:O6   | 48:WA:3773:C:N4    | 2.45                     | 0.50              |
| 48:WA:4262:U:H2'  | 48:WA:4263:C:H6    | 1.75                     | 0.50              |
| 48:WA:4977:G:O2'  | 48:WA:4979:A:N6    | 2.42                     | 0.50              |
| 51:ZA:1605:G:H2'  | 51:ZA:1606:G:C4    | 2.47                     | 0.50              |
| 70:SB:105:ASN:OD1 | 70:SB:108:ARG:NH2  | 2.41                     | 0.50              |
| 74:WB:80:ASP:OD1  | 74:WB:124:LYS:NZ   | 2.45                     | 0.50              |
| 6:F:33:ARG:NH1    | 48:WA:1274:C:OP2   | 2.45                     | 0.49              |
| 30:DA:44:ARG:NH2  | 30:DA:52:GLN:OE1   | 2.45                     | 0.49              |
| 43:RA:117:ARG:HG3 | 43:RA:125:LEU:HD11 | 1.94                     | 0.49              |
| 45:TA:9:A:O2'     | 45:TA:10:G:N7      | 2.37                     | 0.49              |
| 48:WA:4190:U:H2'  | 48:WA:4191:U:C6    | 2.47                     | 0.49              |
| 50:YA:9:A:H2'     | 50:YA:10:G:H8      | 1.77                     | 0.49              |
| 51:ZA:582:U:OP1   | 61:JB:162:ARG:NH1  | 2.45                     | 0.49              |
| 51:ZA:1558:C:H2'  | 51:ZA:1559:C:C6    | 2.47                     | 0.49              |
| 52:AB:176:TRP:NE1 | 52:AB:197:VAL:O    | 2.42                     | 0.49              |
| 78:AC:44:ILE:HG23 | 78:AC:45:VAL:HG23  | 1.94                     | 0.49              |
| 6:F:56:TYR:OH     | 6:F:188:ASP:OD1    | 2.28                     | 0.49              |
| 23:W:139:ARG:HH12 | 48:WA:2535:C:H5''  | 1.76                     | 0.49              |
| 25:Y:47:ASP:N     | 25:Y:69:LYS:O      | 2.43                     | 0.49              |
| 25:Y:50:PRO:HD3   | 25:Y:68:ILE:HG13   | 1.93                     | 0.49              |
| 28:BA:79:ILE:HG12 | 28:BA:90:ARG:HG2   | 1.94                     | 0.49              |
| 45:TA:21:A:N1     | 45:TA:46:G:O2'     | 2.43                     | 0.49              |
| 48:WA:2311:G:O2'  | 50:YA:18:U:O2      | 2.30                     | 0.49              |
| 52:AB:190:SER:OG  | 52:AB:192:GLU:OE1  | 2.29                     | 0.49              |
| 54:CB:192:LEU:HB3 | 54:CB:227:ARG:HB3  | 1.94                     | 0.49              |
| 76:YB:27:VAL:HG12 | 76:YB:29:HIS:HD2   | 1.77                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 86:b:128:THR:OG1   | 86:b:129:GLY:N     | 2.40                     | 0.49              |
| 1:A:236:GLY:N      | 48:WA:3689:A:O2'   | 2.45                     | 0.49              |
| 12:L:41:PRO:HG3    | 12:L:73:VAL:HG12   | 1.95                     | 0.49              |
| 30:DA:100:ALA:O    | 30:DA:108:ARG:NH2  | 2.45                     | 0.49              |
| 37:KA:45:ARG:HH21  | 48:WA:2798:G:H5'   | 1.77                     | 0.49              |
| 51:ZA:931:C:H2'    | 51:ZA:932:G:C8     | 2.47                     | 0.49              |
| 54:CB:104:ASP:HB3  | 54:CB:130:ILE:HG13 | 1.93                     | 0.49              |
| 59:HB:289:ILE:HD12 | 59:HB:417:LYS:HG2  | 1.93                     | 0.49              |
| 86:b:52:VAL:HB     | 86:b:90:PHE:HB2    | 1.93                     | 0.49              |
| 4:D:136:ASP:OD1    | 4:D:136:ASP:N      | 2.45                     | 0.49              |
| 15:O:69:HIS:NE2    | 15:O:139:ASP:O     | 2.36                     | 0.49              |
| 27:AA:28:ARG:HB3   | 48:WA:1807:A:C4    | 2.47                     | 0.49              |
| 46:UA:69:A:H2'     | 46:UA:70:A:H8      | 1.77                     | 0.49              |
| 49:XA:57:C:H2'     | 49:XA:58:A:H8      | 1.78                     | 0.49              |
| 51:ZA:128:U:H3'    | 51:ZA:129:C:H6     | 1.76                     | 0.49              |
| 51:ZA:1023:A:OP2   | 65:NB:124:ARG:NH1  | 2.39                     | 0.49              |
| 51:ZA:1101:U:H2'   | 51:ZA:1102:G:C8    | 2.48                     | 0.49              |
| 51:ZA:1139:C:H42   | 51:ZA:1149:A:H62   | 1.60                     | 0.49              |
| 51:ZA:1277:C:OP1   | 62:KB:51:SER:OG    | 2.28                     | 0.49              |
| 51:ZA:1615:U:O4    | 67:PB:40:ARG:NH2   | 2.45                     | 0.49              |
| 52:AB:89:LYS:NZ    | 69:RB:83:ASN:OD1   | 2.43                     | 0.49              |
| 59:HB:356:ARG:HD3  | 59:HB:359:THR:HG21 | 1.93                     | 0.49              |
| 20:T:90:TYR:O      | 20:T:94:ASN:ND2    | 2.37                     | 0.49              |
| 48:WA:3895:C:H2'   | 48:WA:3896:A:H8    | 1.77                     | 0.49              |
| 51:ZA:822:U:H3     | 51:ZA:826:A:H62    | 1.61                     | 0.49              |
| 56:EB:11:ARG:HA    | 56:EB:28:ALA:HB2   | 1.95                     | 0.49              |
| 71:TB:41:LYS:NZ    | 71:TB:83:GLN:OE1   | 2.44                     | 0.49              |
| 18:R:98:ARG:NH2    | 48:WA:750:G:O6     | 2.45                     | 0.49              |
| 25:Y:25:ILE:HA     | 25:Y:43:VAL:HG12   | 1.93                     | 0.49              |
| 26:Z:65:ARG:NH2    | 48:WA:86:U:HO2'    | 2.10                     | 0.49              |
| 48:WA:2024:C:H5''  | 86:b:83:ARG:HD2    | 1.92                     | 0.49              |
| 51:ZA:639:C:H2'    | 51:ZA:640:A:H8     | 1.77                     | 0.49              |
| 51:ZA:1568:C:OP1   | 71:TB:96:SER:OG    | 2.28                     | 0.49              |
| 51:ZA:1650:A:H5''  | 68:QB:165:ALA:HB2  | 1.95                     | 0.49              |
| 51:ZA:1670:C:H2'   | 51:ZA:1671:G:C8    | 2.47                     | 0.49              |
| 54:CB:72:ASP:OD2   | 54:CB:272:HIS:NE2  | 2.43                     | 0.49              |
| 57:FB:122:ARG:HE   | 80:CC:59:LEU:HD21  | 1.77                     | 0.49              |
| 58:GB:7:PHE:HB3    | 58:GB:10:THR:HG22  | 1.95                     | 0.49              |
| 60:IB:81:VAL:HG22  | 60:IB:102:VAL:HG12 | 1.95                     | 0.49              |
| 4:D:91:GLY:O       | 4:D:94:ASN:ND2     | 2.46                     | 0.49              |
| 8:H:92:MET:HG2     | 8:H:181:VAL:HG22   | 1.95                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:K:64:VAL:HG12  | 48:WA:71:C:H4'    | 1.95                     | 0.49              |
| 22:V:82:ILE:HG12  | 58:GB:131:ARG:HB2 | 1.94                     | 0.49              |
| 35:IA:3:LYS:HB3   | 48:WA:3644:A:C4   | 2.48                     | 0.49              |
| 35:IA:13:ASN:ND2  | 48:WA:1620:G:OP1  | 2.40                     | 0.49              |
| 48:WA:1505:A:H1'  | 48:WA:1506:G:C8   | 2.48                     | 0.49              |
| 48:WA:1751:A:H2'  | 48:WA:1752:G:C8   | 2.48                     | 0.49              |
| 48:WA:1999:U:O2'  | 86:b:44:ARG:NH2   | 2.46                     | 0.49              |
| 51:ZA:106:C:H2'   | 51:ZA:107:A:C8    | 2.46                     | 0.49              |
| 51:ZA:1165:G:OP2  | 51:ZA:1165:G:N2   | 2.36                     | 0.49              |
| 58:GB:48:TYR:OH   | 58:GB:119:LYS:O   | 2.27                     | 0.49              |
| 61:JB:59:GLU:OE2  | 61:JB:69:ARG:NH2  | 2.45                     | 0.49              |
| 64:MB:33:ARG:HD3  | 64:MB:91:LEU:HD22 | 1.94                     | 0.49              |
| 2:B:122:TRP:CH2   | 2:B:127:LYS:HG2   | 2.48                     | 0.49              |
| 2:B:252:ALA:HB1   | 48:WA:4526:G:N3   | 2.28                     | 0.49              |
| 7:G:126:ARG:NE    | 48:WA:4078:G:OP1  | 2.36                     | 0.49              |
| 14:N:94:ARG:HD2   | 48:WA:1311:C:H5'' | 1.94                     | 0.49              |
| 20:T:66:SER:HB3   | 20:T:69:LYS:HB3   | 1.94                     | 0.49              |
| 25:Y:112:ARG:NH2  | 48:WA:2574:C:O2'  | 2.46                     | 0.49              |
| 37:KA:20:ASN:O    | 37:KA:41:ARG:NH1  | 2.45                     | 0.49              |
| 39:MA:15:ARG:NH2  | 51:ZA:1183:A:OP1  | 2.46                     | 0.49              |
| 41:OA:30:GLU:HA   | 41:OA:33:GLN:HG2  | 1.94                     | 0.49              |
| 46:UA:69:A:H2'    | 46:UA:70:A:C8     | 2.47                     | 0.49              |
| 48:WA:1639:A:OP1  | 48:WA:1642:C:N4   | 2.37                     | 0.49              |
| 49:XA:28:C:O2'    | 49:XA:54:A:N1     | 2.46                     | 0.49              |
| 51:ZA:1345:G:OP1  | 51:ZA:1688:C:O2'  | 2.31                     | 0.49              |
| 55:DB:50:VAL:HG21 | 81:DC:34:TYR:HB3  | 1.94                     | 0.49              |
| 58:GB:198:ARG:O   | 58:GB:202:ASN:ND2 | 2.33                     | 0.49              |
| 78:AC:46:GLU:HG3  | 78:AC:48:ALA:H    | 1.78                     | 0.49              |
| 10:J:136:ARG:HG3  | 10:J:157:ILE:HD11 | 1.94                     | 0.49              |
| 13:M:44:ARG:NH1   | 48:WA:280:G:OP2   | 2.40                     | 0.49              |
| 44:SA:22:A:H2'    | 44:SA:23:G:C8     | 2.48                     | 0.49              |
| 48:WA:275:C:H2'   | 48:WA:276:C:C6    | 2.48                     | 0.49              |
| 48:WA:2418:G:N2   | 48:WA:2428:U:O4   | 2.46                     | 0.49              |
| 48:WA:4116:C:H2'  | 48:WA:4117:G:C8   | 2.48                     | 0.49              |
| 48:WA:4652:G:H4'  | 48:WA:5010:C:H4'  | 1.95                     | 0.49              |
| 48:WA:5008:U:H4'  | 48:WA:5009:A:H5'  | 1.93                     | 0.49              |
| 51:ZA:65:C:H4'    | 58:GB:172:LYS:HD3 | 1.94                     | 0.49              |
| 51:ZA:397:G:OP1   | 63:LB:106:HIS:NE2 | 2.46                     | 0.49              |
| 62:KB:11:ILE:HD11 | 62:KB:45:VAL:HG22 | 1.94                     | 0.49              |
| 5:E:67:ARG:NE     | 48:WA:1076:G:OP1  | 2.46                     | 0.49              |
| 11:K:27:ASN:HB3   | 50:YA:29:G:H5''   | 1.95                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 21:U:50:ASN:ND2    | 48:WA:4459:U:OP1   | 2.45                     | 0.49              |
| 25:Y:135:ARG:O     | 48:WA:4124:G:N2    | 2.42                     | 0.49              |
| 28:BA:39:ARG:NH2   | 28:BA:63:TYR:OH    | 2.46                     | 0.49              |
| 48:WA:164:G:H2'    | 48:WA:165:A:H8     | 1.78                     | 0.49              |
| 48:WA:739:C:O2'    | 48:WA:742:G:OP1    | 2.29                     | 0.49              |
| 48:WA:3934:U:H2'   | 48:WA:3935:G:H8    | 1.77                     | 0.49              |
| 48:WA:4194:A:H2'   | 48:WA:4195:C:H6    | 1.78                     | 0.49              |
| 51:ZA:1115:U:O2    | 51:ZA:1116:C:O2'   | 2.31                     | 0.49              |
| 51:ZA:1854:U:OP2   | 66:OB:147:ARG:NH2  | 2.45                     | 0.49              |
| 64:MB:26:LEU:HD22  | 64:MB:33:ARG:HH22  | 1.77                     | 0.49              |
| 84:GC:91:ASP:OD2   | 84:GC:93:THR:OG1   | 2.26                     | 0.49              |
| 88:HC:442:ASP:OD1  | 88:HC:443:LYS:N    | 2.44                     | 0.49              |
| 20:T:56:LEU:HD13   | 20:T:63:LEU:HD13   | 1.93                     | 0.48              |
| 30:DA:64:LYS:NZ    | 48:WA:2081:G:OP2   | 2.36                     | 0.48              |
| 43:RA:37:LEU:HD12  | 43:RA:42:VAL:HB    | 1.95                     | 0.48              |
| 48:WA:3601:A:H2'   | 48:WA:3602:G:H8    | 1.78                     | 0.48              |
| 48:WA:4770:G:O2'   | 48:WA:4875:G:O6    | 2.30                     | 0.48              |
| 51:ZA:1010:G:H2'   | 51:ZA:1011:A:H8    | 1.77                     | 0.48              |
| 57:FB:30:ILE:HB    | 57:FB:36:GLN:HG2   | 1.94                     | 0.48              |
| 58:GB:2:LYS:HD3    | 58:GB:15:LEU:HD21  | 1.94                     | 0.48              |
| 59:HB:304:VAL:HG22 | 59:HB:334:ALA:HB1  | 1.95                     | 0.48              |
| 3:C:192:GLY:O      | 3:C:195:LYS:NZ     | 2.45                     | 0.48              |
| 5:E:96:THR:HG22    | 5:E:109:VAL:HG22   | 1.94                     | 0.48              |
| 18:R:112:ASP:OD1   | 18:R:116:ARG:NH1   | 2.44                     | 0.48              |
| 25:Y:67:LYS:NZ     | 48:WA:2575:A:OP1   | 2.37                     | 0.48              |
| 42:PA:94:ARG:HG3   | 42:PA:107:ARG:HD2  | 1.94                     | 0.48              |
| 48:WA:1176:G:H2'   | 48:WA:1177:G:C8    | 2.48                     | 0.48              |
| 48:WA:1908:U:H2'   | 48:WA:1909:A:H8    | 1.78                     | 0.48              |
| 51:ZA:582:U:H2'    | 51:ZA:583:A:H5''   | 1.95                     | 0.48              |
| 51:ZA:1523:C:H3'   | 70:SB:141:ARG:HH21 | 1.78                     | 0.48              |
| 51:ZA:1693:G:N2    | 51:ZA:1834:A:H8    | 2.11                     | 0.48              |
| 52:AB:164:ASN:O    | 52:AB:170:SER:OG   | 2.22                     | 0.48              |
| 63:LB:38:LYS:NZ    | 63:LB:61:PRO:O     | 2.46                     | 0.48              |
| 83:FC:100:LEU:HD23 | 83:FC:103:LEU:HD23 | 1.96                     | 0.48              |
| 84:GC:4:GLN:HG3    | 84:GC:314:ILE:HG22 | 1.96                     | 0.48              |
| 19:S:70:HIS:N      | 48:WA:4316:C:OP1   | 2.46                     | 0.48              |
| 48:WA:711:G:H2'    | 48:WA:712:A:H8     | 1.78                     | 0.48              |
| 51:ZA:952:G:H2'    | 51:ZA:953:C:C6     | 2.48                     | 0.48              |
| 52:AB:24:HIS:HB3   | 52:AB:51:LEU:HD21  | 1.95                     | 0.48              |
| 61:JB:42:GLU:OE1   | 61:JB:45:ARG:NH2   | 2.45                     | 0.48              |
| 88:HC:282:PRO:HG2  | 88:HC:324:ASN:HA   | 1.94                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 88:HC:287:THR:OG1  | 88:HC:288:GLU:N    | 2.46                     | 0.48              |
| 1:A:21:LYS:HG2     | 48:WA:1543:C:H5''  | 1.95                     | 0.48              |
| 14:N:42:ASN:HD22   | 14:N:125:LYS:HD3   | 1.79                     | 0.48              |
| 14:N:46:ASN:O      | 14:N:50:ASN:ND2    | 2.43                     | 0.48              |
| 48:WA:2560:C:H2'   | 48:WA:2561:G:C8    | 2.49                     | 0.48              |
| 51:ZA:5:U:H2'      | 51:ZA:6:G:C8       | 2.48                     | 0.48              |
| 51:ZA:333:G:H2'    | 51:ZA:334:C:O4'    | 2.14                     | 0.48              |
| 51:ZA:498:C:H2'    | 51:ZA:499:G:C8     | 2.49                     | 0.48              |
| 59:HB:258:GLU:N    | 59:HB:258:GLU:OE1  | 2.47                     | 0.48              |
| 32:FA:24:ARG:NH2   | 48:WA:2615:C:OP1   | 2.46                     | 0.48              |
| 48:WA:1671:A:N3    | 48:WA:1854:U:O2'   | 2.37                     | 0.48              |
| 48:WA:1808:G:H2'   | 48:WA:1809:C:H6    | 1.79                     | 0.48              |
| 48:WA:2575:A:N7    | 48:WA:2763:U:O4    | 2.46                     | 0.48              |
| 51:ZA:1309:C:H5'   | 83:FC:105:TYR:CE1  | 2.49                     | 0.48              |
| 51:ZA:1545:A:OP1   | 68:QB:100:GLY:N    | 2.43                     | 0.48              |
| 6:F:178:LEU:HB3    | 6:F:183:ILE:HB     | 1.95                     | 0.48              |
| 8:H:89:ARG:NH1     | 8:H:147:GLU:OE2    | 2.46                     | 0.48              |
| 16:P:2:GLY:N       | 48:WA:2074:C:OP1   | 2.47                     | 0.48              |
| 16:P:178:ARG:N     | 26:Z:51:GLY:HA2    | 2.29                     | 0.48              |
| 24:X:45:ARG:NH2    | 48:WA:199:G:OP2    | 2.46                     | 0.48              |
| 29:CA:118:GLN:OE1  | 48:WA:5057:G:N2    | 2.46                     | 0.48              |
| 48:WA:711:G:H2'    | 48:WA:712:A:C8     | 2.49                     | 0.48              |
| 48:WA:3879:A:O2'   | 48:WA:4402:G:N2    | 2.47                     | 0.48              |
| 48:WA:4529:G:OP2   | 48:WA:4529:G:N2    | 2.46                     | 0.48              |
| 48:WA:4644:U:H2'   | 48:WA:4645:G:H8    | 1.78                     | 0.48              |
| 51:ZA:1271:C:N4    | 51:ZA:1512:C:N3    | 2.61                     | 0.48              |
| 51:ZA:1656:G:O6    | 51:ZA:1668:U:O4    | 2.31                     | 0.48              |
| 64:MB:32:ALA:HB1   | 64:MB:37:GLU:HB3   | 1.96                     | 0.48              |
| 68:QB:126:VAL:HG12 | 68:QB:127:ASP:H    | 1.79                     | 0.48              |
| 74:WB:11:LEU:HA    | 74:WB:14:ILE:HG12  | 1.95                     | 0.48              |
| 75:XB:90:CYS:HB3   | 75:XB:130:LEU:HD11 | 1.95                     | 0.48              |
| 86:b:60:MET:N      | 86:b:60:MET:SD     | 2.86                     | 0.48              |
| 2:B:108:GLU:OE2    | 2:B:138:GLN:NE2    | 2.44                     | 0.48              |
| 48:WA:287:U:H2'    | 48:WA:288:G:C8     | 2.48                     | 0.48              |
| 48:WA:1874:G:O2'   | 48:WA:4221:A:N3    | 2.47                     | 0.48              |
| 51:ZA:1829:G:H1'   | 51:ZA:1850:A:H2    | 1.79                     | 0.48              |
| 53:BB:179:ASN:HB3  | 53:BB:183:GLU:HB2  | 1.95                     | 0.48              |
| 58:GB:58:LYS:HA    | 58:GB:107:SER:HB2  | 1.95                     | 0.48              |
| 1:A:118:GLU:OE2    | 48:WA:3664:A:O2'   | 2.31                     | 0.48              |
| 6:F:82:VAL:HG22    | 18:R:62:VAL:HA     | 1.95                     | 0.48              |
| 11:K:18:TRP:NE1    | 48:WA:1518:G:O2'   | 2.45                     | 0.48              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 11:K:31:ARG:NH1   | 48:WA:337:U:OP1    | 2.42                     | 0.48              |
| 15:O:111:ARG:NH2  | 48:WA:2364:U:OP1   | 2.46                     | 0.48              |
| 33:GA:76:LYS:O    | 48:WA:136:C:N4     | 2.47                     | 0.48              |
| 42:PA:28:GLU:HB2  | 42:PA:31:ASN:HB2   | 1.94                     | 0.48              |
| 42:PA:39:ARG:NH1  | 48:WA:2268:C:O2'   | 2.46                     | 0.48              |
| 46:UA:47:U:O2'    | 46:UA:50:U:OP1     | 2.25                     | 0.48              |
| 48:WA:197:A:N1    | 48:WA:225:G:O2'    | 2.39                     | 0.48              |
| 48:WA:655:C:H2'   | 48:WA:656:C:H6     | 1.79                     | 0.48              |
| 48:WA:1095:G:H2'  | 48:WA:1096:G:C8    | 2.48                     | 0.48              |
| 48:WA:2335:G:OP1  | 50:YA:20:A:O2'     | 2.32                     | 0.48              |
| 48:WA:4350:A:O2'  | 48:WA:4352:C:OP2   | 2.29                     | 0.48              |
| 51:ZA:373:G:OP1   | 63:LB:137:THR:OG1  | 2.28                     | 0.48              |
| 51:ZA:1203:G:H2'  | 51:ZA:1204:A:H8    | 1.76                     | 0.48              |
| 51:ZA:1485:U:OP1  | 55:DB:189:LYS:NZ   | 2.46                     | 0.48              |
| 51:ZA:1536:G:H2'  | 51:ZA:1537:A:C8    | 2.49                     | 0.48              |
| 80:CC:12:ALA:HB1  | 80:CC:32:VAL:HB    | 1.96                     | 0.48              |
| 4:D:156:GLY:HA2   | 4:D:181:PRO:HD3    | 1.95                     | 0.48              |
| 14:N:12:ARG:HD3   | 14:N:37:ARG:HH11   | 1.78                     | 0.48              |
| 35:IA:54:LYS:O    | 35:IA:58:THR:HB    | 2.14                     | 0.48              |
| 42:PA:12:ASN:OD1  | 42:PA:19:LYS:NZ    | 2.46                     | 0.48              |
| 48:WA:1496:U:H2'  | 48:WA:1497:G:C8    | 2.49                     | 0.48              |
| 48:WA:3612:A:O2'  | 60:IB:92:ARG:NH2   | 2.47                     | 0.48              |
| 48:WA:4324:G:N2   | 48:WA:4327:A:OP2   | 2.40                     | 0.48              |
| 48:WA:4706:C:H2'  | 48:WA:4707:A:C8    | 2.49                     | 0.48              |
| 48:WA:4725:A:H2'  | 48:WA:4726:A:C8    | 2.49                     | 0.48              |
| 51:ZA:544:G:H2'   | 51:ZA:545:A:C8     | 2.49                     | 0.48              |
| 51:ZA:1712:A:H2'  | 51:ZA:1713:C:C6    | 2.49                     | 0.48              |
| 53:BB:136:ARG:HB2 | 53:BB:218:LEU:HD11 | 1.96                     | 0.48              |
| 64:MB:97:GLU:O    | 64:MB:101:ARG:NH2  | 2.45                     | 0.48              |
| 71:TB:7:LYS:HA    | 71:TB:11:GLN:HE22  | 1.78                     | 0.48              |
| 1:A:67:TYR:OH     | 48:WA:4089:G:N7    | 2.43                     | 0.48              |
| 2:B:124:LYS:NZ    | 48:WA:5065:G:O6    | 2.45                     | 0.48              |
| 5:E:71:TYR:HA     | 5:E:74:LYS:HE2     | 1.96                     | 0.48              |
| 7:G:97:ASP:OD1    | 7:G:98:ILE:N       | 2.45                     | 0.48              |
| 11:K:60:ARG:NH2   | 11:K:67:HIS:O      | 2.46                     | 0.48              |
| 37:KA:3:SER:O     | 48:WA:2783:G:O2'   | 2.32                     | 0.48              |
| 48:WA:2494:C:H2'  | 48:WA:2495:G:C8    | 2.49                     | 0.48              |
| 48:WA:2557:G:H2'  | 48:WA:2558:G:H8    | 1.78                     | 0.48              |
| 48:WA:2610:G:H2'  | 48:WA:2611:G:H8    | 1.78                     | 0.48              |
| 48:WA:4275:A:H2'  | 48:WA:4276:A:C8    | 2.49                     | 0.48              |
| 48:WA:4608:G:O2'  | 88:HC:430:ARG:NH2  | 2.46                     | 0.48              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 51:ZA:564:A:H2'   | 51:ZA:565:G:O4'    | 2.14                     | 0.48              |
| 84:GC:226:HIS:NE2 | 84:GC:229:THR:OG1  | 2.45                     | 0.48              |
| 1:A:243:THR:N     | 48:WA:3747:U:O2'   | 2.43                     | 0.47              |
| 9:I:42:LYS:HB2    | 9:I:45:GLU:HG3     | 1.96                     | 0.47              |
| 10:J:40:LEU:HD12  | 10:J:70:VAL:HG22   | 1.96                     | 0.47              |
| 23:W:65:ALA:HB2   | 33:GA:69:LEU:HD11  | 1.96                     | 0.47              |
| 43:RA:46:ILE:HD11 | 43:RA:62:LEU:HD21  | 1.96                     | 0.47              |
| 51:ZA:1797:U:H2'  | 51:ZA:1798:C:C6    | 2.49                     | 0.47              |
| 51:ZA:1854:U:H2'  | 51:ZA:1855:G:H8    | 1.79                     | 0.47              |
| 69:RB:32:LYS:HD2  | 69:RB:47:ARG:HH11  | 1.78                     | 0.47              |
| 76:YB:103:SER:HB3 | 76:YB:106:GLN:HG2  | 1.96                     | 0.47              |
| 5:E:160:HIS:HB3   | 5:E:163:LYS:HD2    | 1.96                     | 0.47              |
| 7:G:90:LYS:NZ     | 48:WA:4128:C:OP1   | 2.47                     | 0.47              |
| 26:Z:2:PRO:HG3    | 48:WA:1511:C:H5''  | 1.96                     | 0.47              |
| 36:JA:24:LYS:NZ   | 48:WA:2698:A:N1    | 2.44                     | 0.47              |
| 40:NA:52:THR:HG22 | 48:WA:43:U:H4'     | 1.96                     | 0.47              |
| 48:WA:164:G:H2'   | 48:WA:165:A:C8     | 2.49                     | 0.47              |
| 48:WA:470:A:H62   | 48:WA:685:G:H21    | 1.62                     | 0.47              |
| 48:WA:692:C:H2'   | 48:WA:693:A:C8     | 2.50                     | 0.47              |
| 48:WA:2081:G:H2'  | 48:WA:2082:U:C6    | 2.49                     | 0.47              |
| 48:WA:3719:A:H2'  | 48:WA:3720:A:C8    | 2.49                     | 0.47              |
| 48:WA:4588:G:O6   | 48:WA:4719:A:N6    | 2.47                     | 0.47              |
| 51:ZA:442:C:N4    | 51:ZA:449:A:H62    | 2.11                     | 0.47              |
| 51:ZA:1358:U:OP2  | 54:CB:123:ARG:NH2  | 2.48                     | 0.47              |
| 64:MB:49:LEU:HB3  | 64:MB:111:VAL:HG13 | 1.95                     | 0.47              |
| 11:K:138:ASP:OD1  | 33:GA:117:ARG:NH2  | 2.43                     | 0.47              |
| 28:BA:38:ILE:HG21 | 28:BA:63:TYR:HB3   | 1.95                     | 0.47              |
| 35:IA:12:ARG:NH2  | 48:WA:1619:G:O3'   | 2.48                     | 0.47              |
| 48:WA:162:A:H2'   | 48:WA:163:A:H8     | 1.79                     | 0.47              |
| 48:WA:1872:C:H2'  | 48:WA:1873:A:H8    | 1.79                     | 0.47              |
| 48:WA:4165:U:H5'  | 48:WA:4166:C:H5''  | 1.96                     | 0.47              |
| 48:WA:4509:A:H2'  | 48:WA:4510:C:C6    | 2.49                     | 0.47              |
| 48:WA:4950:C:OP2  | 48:WA:4951:G:O2'   | 2.25                     | 0.47              |
| 49:XA:11:A:N1     | 49:XA:66:G:O2'     | 2.46                     | 0.47              |
| 49:XA:62:U:O2'    | 49:XA:64:G:O4'     | 2.32                     | 0.47              |
| 51:ZA:1528:G:H2'  | 51:ZA:1529:C:C6    | 2.50                     | 0.47              |
| 51:ZA:1568:C:H2'  | 51:ZA:1569:A:C8    | 2.50                     | 0.47              |
| 52:AB:2:SER:HB3   | 52:AB:59:LEU:HG    | 1.97                     | 0.47              |
| 75:XB:91:LEU:HD23 | 82:EC:82:VAL:HG21  | 1.97                     | 0.47              |
| 84:GC:62:HIS:ND1  | 84:GC:84:ASP:OD2   | 2.47                     | 0.47              |
| 87:c:247:ASP:HB2  | 88:HC:383:SER:N    | 2.30                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:Y:3:LYS:NZ      | 28:BA:40:GLN:O     | 2.40                     | 0.47              |
| 40:NA:58:LYS:NZ    | 48:WA:4382:A:OP1   | 2.40                     | 0.47              |
| 51:ZA:1113:A:H2'   | 51:ZA:1114:U:C6    | 2.49                     | 0.47              |
| 52:AB:122:LEU:HB2  | 52:AB:142:LEU:HD21 | 1.96                     | 0.47              |
| 59:HB:285:ALA:HB3  | 59:HB:301:PHE:HB2  | 1.97                     | 0.47              |
| 64:MB:42:LEU:O     | 64:MB:72:HIS:ND1   | 2.47                     | 0.47              |
| 77:ZB:73:VAL:HG21  | 77:ZB:88:LEU:HD11  | 1.97                     | 0.47              |
| 25:Y:12:LEU:HB2    | 25:Y:81:MET:HB3    | 1.96                     | 0.47              |
| 26:Z:71:PRO:HG2    | 26:Z:108:TYR:HA    | 1.96                     | 0.47              |
| 36:JA:47:ILE:HG22  | 36:JA:49:ASP:H     | 1.79                     | 0.47              |
| 44:SA:13:U:O2      | 44:SA:23:G:N2      | 2.44                     | 0.47              |
| 48:WA:2413:C:H2'   | 48:WA:2414:A:C8    | 2.50                     | 0.47              |
| 48:WA:2589:A:OP2   | 48:WA:2590:C:N4    | 2.47                     | 0.47              |
| 51:ZA:153:G:N2     | 58:GB:13:GLN:OE1   | 2.38                     | 0.47              |
| 51:ZA:1093:A:H2'   | 51:ZA:1094:C:C6    | 2.49                     | 0.47              |
| 53:BB:86:LEU:HB3   | 53:BB:98:THR:HB    | 1.97                     | 0.47              |
| 59:HB:338:ILE:HG12 | 59:HB:363:VAL:HG11 | 1.95                     | 0.47              |
| 88:HC:266:ARG:NH1  | 88:HC:268:GLU:OE2  | 2.47                     | 0.47              |
| 2:B:224:LYS:HG2    | 2:B:340:THR:HB     | 1.97                     | 0.47              |
| 2:B:240:LEU:HB3    | 2:B:244:THR:HG21   | 1.96                     | 0.47              |
| 4:D:146:LEU:HD21   | 4:D:159:VAL:HG22   | 1.96                     | 0.47              |
| 7:G:106:ARG:NH1    | 48:WA:4165:U:OP1   | 2.46                     | 0.47              |
| 14:N:113:ASP:OD1   | 14:N:114:LYS:N     | 2.48                     | 0.47              |
| 45:TA:7:A:O2'      | 45:TA:49:C:OP2     | 2.32                     | 0.47              |
| 48:WA:4494:U:O2'   | 48:WA:4514:U:O2    | 2.25                     | 0.47              |
| 51:ZA:476:A:N3     | 51:ZA:488:U:O2'    | 2.41                     | 0.47              |
| 51:ZA:551:U:H2'    | 51:ZA:552:G:C8     | 2.49                     | 0.47              |
| 51:ZA:1401:A:H2'   | 51:ZA:1402:A:H8    | 1.79                     | 0.47              |
| 52:AB:108:PHE:HB2  | 52:AB:136:GLU:HB3  | 1.97                     | 0.47              |
| 57:FB:102:LEU:HG   | 77:ZB:110:THR:HG21 | 1.97                     | 0.47              |
| 60:IB:67:TRP:NE1   | 60:IB:191:GLU:OE2  | 2.41                     | 0.47              |
| 1:A:30:ARG:NH1     | 1:A:33:ASP:OD2     | 2.47                     | 0.47              |
| 4:D:65:ALA:HB2     | 4:D:74:ILE:HD13    | 1.97                     | 0.47              |
| 5:E:141:ARG:NH1    | 5:E:172:SER:O      | 2.47                     | 0.47              |
| 14:N:130:LYS:NZ    | 48:WA:2057:G:O5'   | 2.48                     | 0.47              |
| 15:O:96:VAL:HB     | 15:O:109:GLN:HE21  | 1.78                     | 0.47              |
| 20:T:35:ASP:HB2    | 20:T:38:ASN:HB3    | 1.97                     | 0.47              |
| 48:WA:652:C:H2'    | 48:WA:653:G:C8     | 2.49                     | 0.47              |
| 48:WA:1606:G:H2'   | 48:WA:1607:G:C8    | 2.50                     | 0.47              |
| 48:WA:2896:A:H2'   | 48:WA:2897:A:C8    | 2.50                     | 0.47              |
| 48:WA:3635:C:H2'   | 48:WA:3636:G:C8    | 2.50                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 48:WA:3723:U:H2'  | 48:WA:3724:G:H8   | 1.80                     | 0.47              |
| 48:WA:4575:G:N2   | 48:WA:4724:G:OP2  | 2.48                     | 0.47              |
| 51:ZA:610:G:H2'   | 51:ZA:611:G:H8    | 1.79                     | 0.47              |
| 51:ZA:991:G:N7    | 78:AC:7:ASN:ND2   | 2.62                     | 0.47              |
| 51:ZA:1049:A:O2'  | 51:ZA:1854:U:O2   | 2.33                     | 0.47              |
| 51:ZA:1755:C:H2'  | 51:ZA:1756:C:C6   | 2.50                     | 0.47              |
| 86:b:59:THR:OG1   | 86:b:60:MET:SD    | 2.73                     | 0.47              |
| 1:A:183:GLY:HA2   | 48:WA:1615:A:H5'  | 1.97                     | 0.47              |
| 1:A:207:VAL:HG13  | 1:A:208:GLU:HG3   | 1.96                     | 0.47              |
| 2:B:228:TYR:O     | 48:WA:2837:A:O2'  | 2.31                     | 0.47              |
| 4:D:126:THR:HG22  | 4:D:128:ASP:H     | 1.79                     | 0.47              |
| 45:TA:23:A:H2'    | 45:TA:24:G:C8     | 2.50                     | 0.47              |
| 48:WA:1428:G:N1   | 48:WA:1460:C:OP2  | 2.35                     | 0.47              |
| 48:WA:1813:G:H2'  | 48:WA:1814:C:H6   | 1.80                     | 0.47              |
| 48:WA:2813:G:N1   | 48:WA:2816:C:OP2  | 2.36                     | 0.47              |
| 48:WA:3598:A:H61  | 63:LB:2:ALA:HA    | 1.79                     | 0.47              |
| 51:ZA:1093:A:O3'  | 74:WB:28:ARG:NH2  | 2.47                     | 0.47              |
| 51:ZA:1745:A:H62  | 51:ZA:1789:G:N2   | 2.13                     | 0.47              |
| 52:AB:109:THR:OG1 | 52:AB:136:GLU:OE1 | 2.25                     | 0.47              |
| 53:BB:144:LYS:HD3 | 53:BB:208:HIS:HB3 | 1.96                     | 0.47              |
| 59:HB:258:GLU:HG3 | 59:HB:286:ALA:HB3 | 1.95                     | 0.47              |
| 62:KB:83:LEU:HB3  | 62:KB:85:LEU:HD23 | 1.97                     | 0.47              |
| 67:PB:81:ARG:NH1  | 67:PB:120:SER:OG  | 2.45                     | 0.47              |
| 7:G:191:ALA:O     | 7:G:195:THR:OG1   | 2.29                     | 0.47              |
| 10:J:46:GLN:NE2   | 10:J:73:THR:O     | 2.44                     | 0.47              |
| 13:M:185:GLY:HA2  | 48:WA:78:U:H5''   | 1.97                     | 0.47              |
| 48:WA:2522:C:H2'  | 48:WA:2523:G:C8   | 2.48                     | 0.47              |
| 48:WA:4631:U:H2'  | 48:WA:4632:G:H8   | 1.80                     | 0.47              |
| 51:ZA:77:A:H2     | 58:GB:175:LYS:HG3 | 1.80                     | 0.47              |
| 51:ZA:155:G:H4'   | 58:GB:15:LEU:HD22 | 1.97                     | 0.47              |
| 51:ZA:348:A:H2'   | 51:ZA:349:A:C8    | 2.50                     | 0.47              |
| 51:ZA:917:U:H2'   | 51:ZA:918:U:C6    | 2.49                     | 0.47              |
| 57:FB:122:ARG:N   | 57:FB:197:GLU:OE2 | 2.41                     | 0.47              |
| 66:OB:146:ARG:HG3 | 78:AC:29:CYS:HB2  | 1.97                     | 0.47              |
| 74:WB:18:GLU:HG3  | 74:WB:69:LEU:HD23 | 1.97                     | 0.47              |
| 76:YB:102:THR:OG1 | 76:YB:107:ARG:NH2 | 2.47                     | 0.47              |
| 3:C:152:LEU:HD23  | 3:C:251:ILE:HG12  | 1.97                     | 0.47              |
| 4:D:54:ARG:NH2    | 4:D:147:ASP:OD2   | 2.47                     | 0.47              |
| 6:F:55:HIS:NE2    | 6:F:59:GLU:OE2    | 2.47                     | 0.47              |
| 14:N:85:ARG:HG3   | 14:N:99:LEU:HD11  | 1.97                     | 0.47              |
| 16:P:133:GLY:O    | 16:P:136:THR:OG1  | 2.26                     | 0.47              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 48:WA:1516:U:H2'  | 48:WA:1517:A:C8    | 2.50                     | 0.47              |
| 48:WA:2542:C:H2'  | 48:WA:2543:G:H8    | 1.80                     | 0.47              |
| 48:WA:4262:U:H2'  | 48:WA:4263:C:C6    | 2.50                     | 0.47              |
| 48:WA:4423:C:N4   | 48:WA:4477:G:H22   | 2.10                     | 0.47              |
| 48:WA:4929:G:H5'' | 48:WA:4930:C:H5    | 1.80                     | 0.47              |
| 51:ZA:128:U:H3'   | 51:ZA:129:C:C6     | 2.49                     | 0.47              |
| 51:ZA:322:C:H2'   | 51:ZA:323:C:H5''   | 1.96                     | 0.47              |
| 51:ZA:1781:A:H2'  | 51:ZA:1782:G:H8    | 1.80                     | 0.47              |
| 54:CB:196:ILE:HB  | 54:CB:223:TYR:HB2  | 1.97                     | 0.47              |
| 59:HB:268:LEU:O   | 59:HB:272:SER:OG   | 2.26                     | 0.47              |
| 4:D:53:VAL:HG11   | 4:D:159:VAL:HA     | 1.97                     | 0.46              |
| 5:E:144:ARG:NH1   | 31:EA:110:ILE:OXT  | 2.39                     | 0.46              |
| 5:E:184:LEU:O     | 48:WA:4885:C:N4    | 2.47                     | 0.46              |
| 16:P:175:GLU:OE2  | 26:Z:49:HIS:ND1    | 2.45                     | 0.46              |
| 25:Y:136:PHE:OXT  | 48:WA:4124:G:O2'   | 2.30                     | 0.46              |
| 31:EA:50:VAL:HG22 | 31:EA:69:VAL:HG22  | 1.96                     | 0.46              |
| 48:WA:1825:G:H2'  | 48:WA:1826:G:C8    | 2.50                     | 0.46              |
| 48:WA:2751:C:H2'  | 48:WA:2752:G:H8    | 1.79                     | 0.46              |
| 51:ZA:196:C:H2'   | 51:ZA:197:U:C6     | 2.51                     | 0.46              |
| 51:ZA:1309:C:H5'  | 83:FC:105:TYR:HE1  | 1.80                     | 0.46              |
| 53:BB:146:ARG:HB2 | 53:BB:149:GLN:HB2  | 1.97                     | 0.46              |
| 55:DB:66:GLU:HG2  | 55:DB:107:LEU:HD21 | 1.98                     | 0.46              |
| 7:G:213:ASP:OD1   | 7:G:213:ASP:N      | 2.48                     | 0.46              |
| 15:O:151:ALA:HB3  | 15:O:172:PRO:HG2   | 1.98                     | 0.46              |
| 16:P:121:LEU:HD22 | 16:P:125:GLN:HG2   | 1.96                     | 0.46              |
| 28:BA:103:ASP:HB3 | 28:BA:106:ARG:HH21 | 1.80                     | 0.46              |
| 48:WA:1306:C:H2'  | 48:WA:1307:C:C6    | 2.51                     | 0.46              |
| 48:WA:2599:G:H2'  | 48:WA:2600:A:C8    | 2.50                     | 0.46              |
| 49:XA:12:U:OP2    | 49:XA:67:C:O2'     | 2.33                     | 0.46              |
| 51:ZA:65:C:OP1    | 58:GB:136:LYS:NZ   | 2.46                     | 0.46              |
| 51:ZA:527:C:H2'   | 51:ZA:528:A:C8     | 2.49                     | 0.46              |
| 51:ZA:694:G:N1    | 51:ZA:732:U:O4     | 2.48                     | 0.46              |
| 63:LB:50:ALA:HA   | 63:LB:55:TYR:HE1   | 1.80                     | 0.46              |
| 65:NB:29:THR:OG1  | 65:NB:31:ASP:OD1   | 2.30                     | 0.46              |
| 3:C:7:LEU:HB3     | 3:C:21:ASN:HB3     | 1.98                     | 0.46              |
| 10:J:146:ARG:HG2  | 10:J:147:ARG:HG3   | 1.96                     | 0.46              |
| 18:R:164:LYS:HB2  | 18:R:165:PRO:HD3   | 1.97                     | 0.46              |
| 19:S:44:GLY:HA2   | 19:S:95:HIS:HB3    | 1.97                     | 0.46              |
| 23:W:120:ASP:N    | 23:W:120:ASP:OD1   | 2.47                     | 0.46              |
| 48:WA:2082:U:H2'  | 48:WA:2083:C:C6    | 2.50                     | 0.46              |
| 48:WA:2581:G:N2   | 48:WA:2584:A:OP2   | 2.30                     | 0.46              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 48:WA:3719:A:H2'  | 48:WA:3720:A:H8    | 1.80                     | 0.46              |
| 51:ZA:671:A:H4'   | 51:ZA:672:A:H5''   | 1.98                     | 0.46              |
| 51:ZA:1217:A:H2'  | 51:ZA:1218:C:C6    | 2.50                     | 0.46              |
| 51:ZA:1828:C:H2'  | 51:ZA:1829:G:C8    | 2.50                     | 0.46              |
| 71:TB:116:ASP:OD1 | 71:TB:117:GLN:N    | 2.49                     | 0.46              |
| 88:HC:272:LEU:HB3 | 88:HC:302:ALA:HB3  | 1.98                     | 0.46              |
| 16:P:37:ARG:NH1   | 48:WA:2089:C:OP2   | 2.47                     | 0.46              |
| 31:EA:46:ARG:HD3  | 31:EA:106:TYR:HD2  | 1.78                     | 0.46              |
| 39:MA:11:ARG:NH2  | 51:ZA:1844:U:OP1   | 2.41                     | 0.46              |
| 48:WA:181:C:H2'   | 48:WA:182:G:H8     | 1.78                     | 0.46              |
| 48:WA:2745:A:H2'  | 48:WA:2746:A:C8    | 2.51                     | 0.46              |
| 48:WA:3912:C:H2'  | 48:WA:3913:C:H6    | 1.80                     | 0.46              |
| 48:WA:4128:C:H5'' | 48:WA:4129:A:H5''  | 1.97                     | 0.46              |
| 48:WA:4929:G:H5'' | 48:WA:4930:C:C5    | 2.50                     | 0.46              |
| 50:YA:47:C:H1'    | 50:YA:61:A:H2'     | 1.97                     | 0.46              |
| 51:ZA:10:G:O2'    | 54:CB:113:GLN:OE1  | 2.32                     | 0.46              |
| 51:ZA:1103:C:H2'  | 51:ZA:1104:G:C8    | 2.50                     | 0.46              |
| 51:ZA:1447:G:H2'  | 51:ZA:1448:A:C8    | 2.51                     | 0.46              |
| 86:b:47:LEU:HD13  | 86:b:51:ALA:HB3    | 1.98                     | 0.46              |
| 2:B:213:GLN:NE2   | 2:B:285:TYR:O      | 2.49                     | 0.46              |
| 8:H:18:ILE:HG12   | 8:H:27:VAL:HG22    | 1.96                     | 0.46              |
| 12:L:29:ASP:OD1   | 12:L:30:VAL:N      | 2.48                     | 0.46              |
| 31:EA:21:GLN:NE2  | 48:WA:1311:C:O2    | 2.49                     | 0.46              |
| 40:NA:3:ASN:HA    | 40:NA:92:GLU:HG3   | 1.96                     | 0.46              |
| 48:WA:478:G:H2'   | 48:WA:479:G:H8     | 1.80                     | 0.46              |
| 48:WA:1330:G:O2'  | 48:WA:2351:A:OP1   | 2.34                     | 0.46              |
| 48:WA:2377:A:H2'  | 48:WA:2378:A:C8    | 2.48                     | 0.46              |
| 48:WA:3725:A:H2'  | 48:WA:3726:A:C8    | 2.51                     | 0.46              |
| 64:MB:33:ARG:HH11 | 64:MB:91:LEU:HD13  | 1.80                     | 0.46              |
| 6:F:156:ARG:NH2   | 48:WA:2075:C:O2'   | 2.49                     | 0.46              |
| 8:H:95:VAL:HB     | 38:LA:56:LEU:HB3   | 1.96                     | 0.46              |
| 9:I:31:ILE:HB     | 9:I:66:GLU:HB2     | 1.98                     | 0.46              |
| 17:Q:84:THR:HG22  | 48:WA:2866:A:H5''  | 1.97                     | 0.46              |
| 20:T:19:LEU:HD22  | 20:T:78:PHE:H      | 1.80                     | 0.46              |
| 30:DA:89:LEU:HD13 | 30:DA:118:LEU:HD22 | 1.96                     | 0.46              |
| 30:DA:104:SER:HB2 | 48:WA:2305:C:H5''  | 1.98                     | 0.46              |
| 34:HA:70:LEU:HD13 | 34:HA:87:ARG:HE    | 1.81                     | 0.46              |
| 46:UA:17:G:HO2'   | 46:UA:57:G:H22     | 1.60                     | 0.46              |
| 48:WA:1295:G:OP2  | 48:WA:1295:G:N2    | 2.34                     | 0.46              |
| 48:WA:2541:C:H2'  | 48:WA:2542:C:C6    | 2.51                     | 0.46              |
| 48:WA:4690:C:H2'  | 48:WA:4691:U:C6    | 2.51                     | 0.46              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 51:ZA:1798:C:H2'  | 51:ZA:1799:G:O4'   | 2.16                     | 0.46              |
| 54:CB:201:GLY:O   | 61:JB:54:ARG:NH1   | 2.49                     | 0.46              |
| 60:IB:131:PRO:HD2 | 60:IB:134:GLU:HB2  | 1.97                     | 0.46              |
| 71:TB:96:SER:HB3  | 71:TB:99:VAL:HG22  | 1.97                     | 0.46              |
| 84:GC:124:SER:OG  | 84:GC:125:ARG:N    | 2.49                     | 0.46              |
| 15:O:66:LYS:NZ    | 48:WA:425:U:OP1    | 2.42                     | 0.46              |
| 48:WA:128:C:H2'   | 48:WA:129:C:C6     | 2.51                     | 0.46              |
| 48:WA:262:G:H2'   | 48:WA:263:G:H8     | 1.78                     | 0.46              |
| 48:WA:306:A:H2'   | 48:WA:307:A:C8     | 2.51                     | 0.46              |
| 48:WA:1263:G:H2'  | 48:WA:1264:G:C8    | 2.50                     | 0.46              |
| 48:WA:2745:A:H2'  | 48:WA:2746:A:H8    | 1.80                     | 0.46              |
| 48:WA:3952:U:H2'  | 48:WA:3953:G:C8    | 2.51                     | 0.46              |
| 48:WA:4110:G:H2'  | 48:WA:4111:G:C8    | 2.49                     | 0.46              |
| 50:YA:45:C:H2'    | 50:YA:46:G:H8      | 1.81                     | 0.46              |
| 51:ZA:326:C:O2    | 51:ZA:327:G:N1     | 2.49                     | 0.46              |
| 58:GB:5:ILE:HD12  | 58:GB:16:ILE:HD13  | 1.97                     | 0.46              |
| 62:KB:16:PHE:HE2  | 62:KB:89:ILE:HG22  | 1.80                     | 0.46              |
| 64:MB:22:LEU:HD13 | 64:MB:89:VAL:HA    | 1.97                     | 0.46              |
| 2:B:234:ARG:NH1   | 2:B:271:GLN:O      | 2.37                     | 0.46              |
| 6:F:130:ASN:ND2   | 48:WA:1729:U:OP1   | 2.48                     | 0.46              |
| 9:I:51:HIS:HD2    | 9:I:168:SER:HB2    | 1.81                     | 0.46              |
| 11:K:54:PRO:HG2   | 11:K:56:ARG:NH1    | 2.30                     | 0.46              |
| 12:L:24:LEU:HD11  | 12:L:86:TRP:CG     | 2.51                     | 0.46              |
| 14:N:37:ARG:HH21  | 14:N:108:ILE:HD11  | 1.81                     | 0.46              |
| 33:GA:62:ASN:ND2  | 50:YA:60:G:O6      | 2.39                     | 0.46              |
| 36:JA:24:LYS:HE2  | 36:JA:69:LEU:HD11  | 1.98                     | 0.46              |
| 48:WA:2701:C:H2'  | 48:WA:2702:G:H8    | 1.80                     | 0.46              |
| 48:WA:4571:U:OP1  | 48:WA:4984:A:O2'   | 2.30                     | 0.46              |
| 51:ZA:12:U:H5''   | 54:CB:110:MET:HE2  | 1.98                     | 0.46              |
| 51:ZA:1406:G:H2'  | 51:ZA:1407:U:H6    | 1.81                     | 0.46              |
| 51:ZA:1431:G:H2'  | 51:ZA:1432:U:C6    | 2.50                     | 0.46              |
| 51:ZA:1524:G:OP2  | 70:SB:141:ARG:NE   | 2.46                     | 0.46              |
| 54:CB:65:LYS:HD2  | 54:CB:273:LEU:HD13 | 1.96                     | 0.46              |
| 72:UB:98:VAL:HG23 | 72:UB:101:ILE:HD11 | 1.98                     | 0.46              |
| 73:VB:59:ILE:HD12 | 79:BC:3:LEU:HD11   | 1.97                     | 0.46              |
| 1:A:27:ALA:O      | 1:A:128:ARG:NH2    | 2.45                     | 0.46              |
| 4:D:94:ASN:OD1    | 4:D:97:ALA:N       | 2.36                     | 0.46              |
| 30:DA:99:ILE:HG21 | 30:DA:108:ARG:HG2  | 1.98                     | 0.46              |
| 30:DA:103:VAL:O   | 30:DA:128:ARG:NH1  | 2.49                     | 0.46              |
| 48:WA:352:G:O2'   | 50:YA:22:U:O4      | 2.30                     | 0.46              |
| 48:WA:2851:A:O2'  | 48:WA:2857:G:N7    | 2.43                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 48:WA:4391:C:H2'   | 48:WA:4392:A:C8    | 2.51                     | 0.46              |
| 51:ZA:1198:G:H2'   | 51:ZA:1199:A:C8    | 2.51                     | 0.46              |
| 52:AB:157:VAL:O    | 73:VB:65:SER:OG    | 2.33                     | 0.46              |
| 69:RB:102:THR:O    | 69:RB:105:MET:HG3  | 2.16                     | 0.46              |
| 1:A:198:ARG:NH2    | 48:WA:3690:U:OP2   | 2.49                     | 0.46              |
| 3:C:119:GLN:NE2    | 48:WA:1352:C:O2    | 2.45                     | 0.46              |
| 11:K:35:ARG:NH2    | 48:WA:337:U:OP1    | 2.49                     | 0.46              |
| 27:AA:110:ALA:HB1  | 48:WA:1273:G:H5'   | 1.98                     | 0.46              |
| 46:UA:17:G:O2'     | 46:UA:57:G:N2      | 2.34                     | 0.46              |
| 48:WA:270:U:H2'    | 48:WA:271:C:C6     | 2.51                     | 0.46              |
| 48:WA:2413:C:H2'   | 48:WA:2414:A:H8    | 1.80                     | 0.46              |
| 48:WA:2626:G:H2'   | 48:WA:2627:U:C6    | 2.52                     | 0.46              |
| 50:YA:153:C:H2'    | 50:YA:154:G:C8     | 2.51                     | 0.46              |
| 51:ZA:516:A:N1     | 51:ZA:643:A:O2'    | 2.46                     | 0.46              |
| 51:ZA:1202:U:H2'   | 51:ZA:1203:G:H8    | 1.81                     | 0.46              |
| 51:ZA:1617:G:N2    | 51:ZA:1619:A:H3'   | 2.31                     | 0.46              |
| 53:BB:103:MET:HE2  | 53:BB:188:LEU:HD11 | 1.98                     | 0.46              |
| 60:IB:26:LYS:O     | 60:IB:29:LEU:HB2   | 2.16                     | 0.46              |
| 88:HC:285:VAL:HG22 | 88:HC:450:LYS:HB3  | 1.97                     | 0.46              |
| 1:A:219:ILE:HD11   | 48:WA:3691:G:H5'   | 1.98                     | 0.45              |
| 2:B:14:LEU:O       | 48:WA:4589:G:O2'   | 2.25                     | 0.45              |
| 46:UA:12:G:H2'     | 46:UA:13:U:O4'     | 2.15                     | 0.45              |
| 48:WA:715:G:H2'    | 48:WA:716:G:H8     | 1.80                     | 0.45              |
| 48:WA:1247:C:H2'   | 48:WA:1248:G:C8    | 2.50                     | 0.45              |
| 48:WA:1292:G:H2'   | 48:WA:1293:G:H8    | 1.81                     | 0.45              |
| 48:WA:1974:G:H2'   | 48:WA:1975:G:O4'   | 2.16                     | 0.45              |
| 48:WA:2310:A:H4'   | 48:WA:2336:C:H4'   | 1.98                     | 0.45              |
| 48:WA:3913:C:H2'   | 48:WA:3914:U:H6    | 1.81                     | 0.45              |
| 48:WA:4321:C:H2'   | 48:WA:4322:G:H8    | 1.81                     | 0.45              |
| 48:WA:4450:G:H5''  | 48:WA:4451:A:H5'   | 1.97                     | 0.45              |
| 48:WA:4460:C:H2'   | 48:WA:4461:U:C6    | 2.51                     | 0.45              |
| 51:ZA:743:U:H3     | 51:ZA:798:G:N2     | 2.14                     | 0.45              |
| 51:ZA:916:A:C5     | 65:NB:73:ARG:HD3   | 2.51                     | 0.45              |
| 74:WB:27:ILE:HG13  | 74:WB:61:ILE:HB    | 1.98                     | 0.45              |
| 4:D:33:ARG:HH21    | 49:XA:7:G:H4'      | 1.81                     | 0.45              |
| 5:E:186:ARG:HG3    | 48:WA:4940:A:H5'   | 1.99                     | 0.45              |
| 9:I:116:ARG:HH12   | 48:WA:4201:C:H42   | 1.63                     | 0.45              |
| 23:W:150:ALA:HB1   | 23:W:155:ILE:HG13  | 1.98                     | 0.45              |
| 29:CA:33:ILE:HD11  | 29:CA:41:ARG:HB3   | 1.98                     | 0.45              |
| 43:RA:137:GLN:HE21 | 43:RA:137:GLN:HB3  | 1.53                     | 0.45              |
| 48:WA:462:G:H2'    | 48:WA:463:A:C8     | 2.52                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 48:WA:1543:C:H1'   | 48:WA:2450:G:H21   | 1.81                     | 0.45              |
| 48:WA:4147:C:H2'   | 48:WA:4148:G:H8    | 1.81                     | 0.45              |
| 51:ZA:618:C:H2'    | 51:ZA:619:A:O4'    | 2.17                     | 0.45              |
| 51:ZA:918:U:O2'    | 74:WB:56:HIS:O     | 2.35                     | 0.45              |
| 72:UB:32:LEU:HD21  | 72:UB:87:ARG:HG2   | 1.98                     | 0.45              |
| 75:XB:51:VAL:HG22  | 75:XB:72:VAL:HG22  | 1.97                     | 0.45              |
| 88:HC:344:VAL:HG12 | 88:HC:436:GLY:HA3  | 1.98                     | 0.45              |
| 4:D:223:PHE:HB3    | 4:D:226:TYR:HB2    | 1.97                     | 0.45              |
| 7:G:253:THR:OG1    | 48:WA:150:U:OP2    | 2.27                     | 0.45              |
| 12:L:47:ARG:HH22   | 12:L:69:ARG:HA     | 1.81                     | 0.45              |
| 16:P:122:THR:OG1   | 16:P:124:ASP:OD1   | 2.27                     | 0.45              |
| 26:Z:75:LEU:HB3    | 26:Z:117:LEU:HD13  | 1.97                     | 0.45              |
| 43:RA:131:GLU:HB2  | 48:WA:1975:G:N2    | 2.31                     | 0.45              |
| 44:SA:43:A:H2'     | 44:SA:44:A:C8      | 2.51                     | 0.45              |
| 48:WA:175:C:H2'    | 48:WA:176:G:H8     | 1.81                     | 0.45              |
| 48:WA:674:C:H2'    | 48:WA:675:G:H8     | 1.81                     | 0.45              |
| 48:WA:910:G:H2'    | 48:WA:911:G:H8     | 1.82                     | 0.45              |
| 51:ZA:107:A:H2'    | 51:ZA:108:G:H8     | 1.80                     | 0.45              |
| 51:ZA:649:U:H2'    | 51:ZA:650:A:C8     | 2.49                     | 0.45              |
| 51:ZA:1778:C:H2'   | 51:ZA:1779:G:C8    | 2.51                     | 0.45              |
| 55:DB:58:GLU:OE2   | 55:DB:114:ARG:NE   | 2.49                     | 0.45              |
| 70:SB:125:HIS:CE1  | 70:SB:131:VAL:HG21 | 2.51                     | 0.45              |
| 10:J:35:ARG:NH1    | 10:J:126:TYR:OH    | 2.49                     | 0.45              |
| 34:HA:60:LEU:HA    | 34:HA:63:VAL:HG22  | 1.97                     | 0.45              |
| 48:WA:1292:G:H2'   | 48:WA:1293:G:C8    | 2.52                     | 0.45              |
| 48:WA:1806:A:H4'   | 48:WA:1807:A:O5'   | 2.15                     | 0.45              |
| 48:WA:1848:G:H2'   | 48:WA:1849:C:C6    | 2.52                     | 0.45              |
| 48:WA:4747:G:H1    | 48:WA:4957:A:N6    | 2.14                     | 0.45              |
| 51:ZA:209:A:H2'    | 51:ZA:210:U:O4'    | 2.16                     | 0.45              |
| 51:ZA:220:U:H2'    | 51:ZA:221:A:H8     | 1.81                     | 0.45              |
| 51:ZA:1716:C:H2'   | 51:ZA:1717:C:H6    | 1.81                     | 0.45              |
| 56:EB:18:TRP:HB3   | 56:EB:20:LEU:HD13  | 1.97                     | 0.45              |
| 56:EB:126:VAL:HA   | 56:EB:141:THR:HA   | 1.98                     | 0.45              |
| 62:KB:26:ASP:HB3   | 62:KB:29:MET:HE3   | 1.98                     | 0.45              |
| 84:GC:107:ASP:N    | 84:GC:107:ASP:OD1  | 2.49                     | 0.45              |
| 1:A:137:ILE:HD11   | 1:A:149:LYS:HB2    | 1.98                     | 0.45              |
| 4:D:146:LEU:HD22   | 4:D:163:LEU:HD13   | 1.97                     | 0.45              |
| 9:I:88:ARG:HH21    | 9:I:173:PHE:HD2    | 1.64                     | 0.45              |
| 16:P:181:ARG:NH2   | 48:WA:4368:A:OP1   | 2.49                     | 0.45              |
| 48:WA:422:C:H2'    | 48:WA:423:G:H8     | 1.81                     | 0.45              |
| 48:WA:425:U:H2'    | 48:WA:426:A:C8     | 2.51                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 48:WA:3609:U:H2'   | 48:WA:3610:A:C8    | 2.51                     | 0.45              |
| 48:WA:4421:U:OP1   | 48:WA:4423:C:N4    | 2.49                     | 0.45              |
| 48:WA:4968:A:H2'   | 48:WA:4969:A:C8    | 2.52                     | 0.45              |
| 51:ZA:527:C:H4'    | 61:JB:121:LYS:HD2  | 1.97                     | 0.45              |
| 51:ZA:562:U:OP1    | 61:JB:134:HIS:NE2  | 2.49                     | 0.45              |
| 51:ZA:613:G:N1     | 51:ZA:629:A:OP2    | 2.50                     | 0.45              |
| 51:ZA:1418:C:N4    | 51:ZA:1422:G:OP1   | 2.50                     | 0.45              |
| 53:BB:137:LEU:HG   | 53:BB:215:VAL:HG22 | 1.97                     | 0.45              |
| 61:JB:114:VAL:HG21 | 61:JB:135:ILE:HD13 | 1.97                     | 0.45              |
| 64:MB:33:ARG:NH2   | 64:MB:89:VAL:O     | 2.49                     | 0.45              |
| 67:PB:43:ARG:HH12  | 67:PB:47:ARG:HH11  | 1.65                     | 0.45              |
| 70:SB:75:ARG:NE    | 70:SB:81:ASP:OD1   | 2.38                     | 0.45              |
| 84:GC:5:MET:HE3    | 84:GC:310:TRP:HB3  | 1.98                     | 0.45              |
| 88:HC:346:ILE:O    | 88:HC:397:GLY:N    | 2.47                     | 0.45              |
| 9:I:61:SER:HA      | 9:I:126:VAL:HG23   | 1.97                     | 0.45              |
| 13:M:53:TYR:HB2    | 13:M:133:ILE:HD13  | 1.99                     | 0.45              |
| 24:X:82:ILE:HD12   | 24:X:85:VAL:HG21   | 1.98                     | 0.45              |
| 30:DA:78:LEU:HB2   | 42:PA:20:ARG:HD2   | 1.99                     | 0.45              |
| 48:WA:146:G:H2'    | 48:WA:147:A:H8     | 1.81                     | 0.45              |
| 48:WA:1343:U:H2'   | 48:WA:1344:A:C8    | 2.51                     | 0.45              |
| 48:WA:1848:G:H2'   | 48:WA:1849:C:H6    | 1.82                     | 0.45              |
| 48:WA:2002:G:O2'   | 48:WA:2003:G:N7    | 2.47                     | 0.45              |
| 48:WA:2609:C:H2'   | 48:WA:2610:G:H8    | 1.82                     | 0.45              |
| 48:WA:2751:C:H2'   | 48:WA:2752:G:C8    | 2.52                     | 0.45              |
| 48:WA:4143:G:N2    | 48:WA:4146:G:OP2   | 2.35                     | 0.45              |
| 51:ZA:1275:G:H22   | 51:ZA:1506:A:P     | 2.39                     | 0.45              |
| 51:ZA:1458:G:OP1   | 84:GC:279:SER:OG   | 2.26                     | 0.45              |
| 62:KB:60:GLU:OE1   | 62:KB:69:TRP:NE1   | 2.41                     | 0.45              |
| 66:OB:31:CYS:HB3   | 66:OB:44:VAL:HG22  | 1.98                     | 0.45              |
| 70:SB:22:GLY:HA2   | 70:SB:56:ALA:HB3   | 1.98                     | 0.45              |
| 84:GC:234:ASP:HB2  | 84:GC:252:THR:HB   | 1.98                     | 0.45              |
| 3:C:333:LYS:NZ     | 48:WA:983:G:O2'    | 2.41                     | 0.45              |
| 9:I:66:GLU:OE1     | 9:I:69:ARG:NH1     | 2.49                     | 0.45              |
| 13:M:184:ILE:HG23  | 13:M:194:ARG:HH22  | 1.82                     | 0.45              |
| 20:T:28:PRO:HB2    | 20:T:34:MET:HG2    | 1.98                     | 0.45              |
| 20:T:84:LYS:HB2    | 20:T:110:TYR:CE2   | 2.51                     | 0.45              |
| 25:Y:54:THR:H      | 25:Y:57:MET:HE2    | 1.82                     | 0.45              |
| 44:SA:21:A:O2'     | 44:SA:22:A:O5'     | 2.25                     | 0.45              |
| 45:TA:49:C:H2'     | 45:TA:50:A:C8      | 2.50                     | 0.45              |
| 48:WA:212:A:H2'    | 48:WA:213:G:H8     | 1.81                     | 0.45              |
| 48:WA:251:C:H2'    | 48:WA:252:C:C6     | 2.52                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 48:WA:986:U:H2'    | 48:WA:987:C:C6     | 2.52                     | 0.45              |
| 48:WA:1944:A:H2'   | 48:WA:1945:A:H8    | 1.81                     | 0.45              |
| 48:WA:2516:G:O2'   | 48:WA:2745:A:N6    | 2.49                     | 0.45              |
| 48:WA:3738:A:H2'   | 48:WA:3739:A:C8    | 2.51                     | 0.45              |
| 51:ZA:1480:A:O2'   | 72:UB:79:ARG:NH2   | 2.49                     | 0.45              |
| 52:AB:127:PRO:HG3  | 52:AB:146:ALA:HB1  | 1.98                     | 0.45              |
| 52:AB:128:ARG:HG2  | 52:AB:153:PRO:HD2  | 1.99                     | 0.45              |
| 59:HB:336:ARG:HD2  | 59:HB:363:VAL:HG23 | 1.99                     | 0.45              |
| 62:KB:37:ASP:N     | 62:KB:37:ASP:OD1   | 2.50                     | 0.45              |
| 84:GC:286:CYS:HA   | 84:GC:302:TYR:HA   | 1.97                     | 0.45              |
| 6:F:222:LYS:HE3    | 48:WA:1909:A:H4'   | 1.99                     | 0.45              |
| 14:N:12:ARG:HB2    | 14:N:37:ARG:HD2    | 1.99                     | 0.45              |
| 16:P:54:SER:OG     | 16:P:57:ASN:OD1    | 2.27                     | 0.45              |
| 17:Q:176:ARG:NH1   | 51:ZA:909:G:OP1    | 2.50                     | 0.45              |
| 48:WA:260:C:H2'    | 48:WA:261:G:C8     | 2.52                     | 0.45              |
| 51:ZA:54:A:OP1     | 76:YB:111:LYS:NZ   | 2.44                     | 0.45              |
| 53:BB:106:THR:HG22 | 53:BB:108:ASP:H    | 1.80                     | 0.45              |
| 58:GB:74:ARG:HG2   | 58:GB:96:SER:HB3   | 1.99                     | 0.45              |
| 63:LB:13:GLN:HB2   | 63:LB:16:ILE:HG12  | 1.97                     | 0.45              |
| 63:LB:45:LYS:HE2   | 63:LB:45:LYS:HB2   | 1.79                     | 0.45              |
| 86:b:16:LYS:HE2    | 86:b:16:LYS:HB3    | 1.64                     | 0.45              |
| 3:C:293:LEU:O      | 3:C:299:GLN:NE2    | 2.46                     | 0.45              |
| 48:WA:36:U:OP1     | 48:WA:1653:G:N2    | 2.40                     | 0.45              |
| 48:WA:677:C:H2'    | 48:WA:678:G:C8     | 2.51                     | 0.45              |
| 48:WA:723:G:OP1    | 48:WA:938:C:N4     | 2.49                     | 0.45              |
| 48:WA:1398:G:O2'   | 48:WA:1470:C:O2'   | 2.31                     | 0.45              |
| 48:WA:1448:C:H2'   | 48:WA:1449:C:C6    | 2.52                     | 0.45              |
| 48:WA:3895:C:H2'   | 48:WA:3896:A:C8    | 2.52                     | 0.45              |
| 48:WA:3925:A:H2'   | 48:WA:3926:C:C6    | 2.51                     | 0.45              |
| 51:ZA:1801:A:H2'   | 51:ZA:1802:C:C6    | 2.51                     | 0.45              |
| 53:BB:99:ASN:OD1   | 53:BB:100:PHE:N    | 2.50                     | 0.45              |
| 54:CB:109:ILE:HD11 | 54:CB:151:ILE:HD11 | 1.99                     | 0.45              |
| 1:A:10:LYS:NZ      | 48:WA:3689:A:OP2   | 2.48                     | 0.45              |
| 3:C:140:LYS:HE3    | 3:C:245:HIS:HB2    | 1.99                     | 0.45              |
| 16:P:79:THR:HB     | 16:P:136:THR:HG22  | 1.98                     | 0.45              |
| 43:RA:47:ALA:O     | 43:RA:50:THR:OG1   | 2.35                     | 0.45              |
| 48:WA:520:C:H2'    | 48:WA:521:U:C5     | 2.52                     | 0.45              |
| 48:WA:2000:A:OP2   | 86:b:16:LYS:NZ     | 2.35                     | 0.45              |
| 48:WA:3873:A:H2'   | 48:WA:3874:A:C8    | 2.51                     | 0.45              |
| 48:WA:4072:U:H2'   | 48:WA:4073:U:C6    | 2.52                     | 0.45              |
| 49:XA:92:C:H2'     | 49:XA:93:G:C8      | 2.48                     | 0.45              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 50:YA:106:G:H4'   | 50:YA:137:A:H5'    | 1.99                     | 0.45              |
| 51:ZA:1440:C:O2'  | 51:ZA:1441:U:O4'   | 2.35                     | 0.45              |
| 51:ZA:1535:U:O4   | 57:FB:159:ARG:NE   | 2.50                     | 0.45              |
| 51:ZA:1614:A:H2'  | 51:ZA:1615:U:C6    | 2.52                     | 0.45              |
| 55:DB:133:GLY:HA2 | 55:DB:139:GLN:HE21 | 1.82                     | 0.45              |
| 55:DB:234:GLY:HA3 | 55:DB:239:LYS:HG2  | 1.97                     | 0.45              |
| 56:EB:95:THR:HG22 | 76:YB:16:ARG:HB2   | 1.99                     | 0.45              |
| 58:GB:39:ASP:N    | 58:GB:39:ASP:OD1   | 2.50                     | 0.45              |
| 70:SB:48:ALA:HB2  | 70:SB:70:ILE:HG13  | 1.98                     | 0.45              |
| 73:VB:11:LEU:HD23 | 73:VB:11:LEU:H     | 1.82                     | 0.45              |
| 75:XB:40:PRO:O    | 75:XB:77:ASN:ND2   | 2.49                     | 0.45              |
| 77:ZB:92:LEU:HD22 | 77:ZB:109:TYR:HE1  | 1.82                     | 0.45              |
| 1:A:227:ARG:NH1   | 48:WA:3667:G:O3'   | 2.50                     | 0.44              |
| 4:D:52:ILE:HD13   | 49:XA:6:C:H4'      | 1.99                     | 0.44              |
| 13:M:14:LYS:HE2   | 48:WA:280:G:H5''   | 1.99                     | 0.44              |
| 19:S:127:GLN:HE21 | 19:S:131:GLN:HE21  | 1.65                     | 0.44              |
| 22:V:20:ARG:HD3   | 22:V:30:GLN:HG3    | 1.99                     | 0.44              |
| 45:TA:52:G:H2'    | 45:TA:53:G:H8      | 1.82                     | 0.44              |
| 48:WA:1307:C:OP1  | 50:YA:7:U:O2'      | 2.35                     | 0.44              |
| 51:ZA:381:C:H41   | 60:IB:27:TYR:HB2   | 1.82                     | 0.44              |
| 51:ZA:570:C:O2'   | 76:YB:34:THR:O     | 2.34                     | 0.44              |
| 51:ZA:1017:U:OP1  | 65:NB:62:GLN:NE2   | 2.41                     | 0.44              |
| 51:ZA:1315:U:H4'  | 62:KB:2:LEU:HB3    | 1.99                     | 0.44              |
| 51:ZA:1643:U:H2'  | 51:ZA:1644:C:C6    | 2.52                     | 0.44              |
| 53:BB:52:THR:HG23 | 53:BB:57:ILE:HG22  | 1.98                     | 0.44              |
| 53:BB:126:ASP:N   | 53:BB:126:ASP:OD1  | 2.50                     | 0.44              |
| 88:HC:363:CYS:HB3 | 88:HC:424:PHE:HB3  | 1.98                     | 0.44              |
| 9:I:87:ILE:HG12   | 9:I:138:ILE:HG12   | 1.99                     | 0.44              |
| 18:R:17:LEU:HD11  | 19:S:136:ARG:HH21  | 1.82                     | 0.44              |
| 19:S:28:ALA:HA    | 19:S:31:MET:HG2    | 1.99                     | 0.44              |
| 19:S:130:ARG:HH21 | 48:WA:1730:U:H1'   | 1.82                     | 0.44              |
| 21:U:82:ILE:HG22  | 21:U:83:ARG:HG3    | 1.99                     | 0.44              |
| 30:DA:124:ASN:N   | 30:DA:124:ASN:OD1  | 2.49                     | 0.44              |
| 37:KA:25:GLN:O    | 37:KA:28:TRP:NE1   | 2.50                     | 0.44              |
| 48:WA:457:G:H1    | 48:WA:700:C:H42    | 1.65                     | 0.44              |
| 48:WA:677:C:H2'   | 48:WA:678:G:H8     | 1.83                     | 0.44              |
| 48:WA:961:A:N6    | 48:WA:1285:G:H1'   | 2.33                     | 0.44              |
| 48:WA:1300:C:H2'  | 48:WA:1301:G:C8    | 2.53                     | 0.44              |
| 48:WA:1492:G:H2'  | 48:WA:1493:A:H8    | 1.82                     | 0.44              |
| 48:WA:1619:G:H1'  | 48:WA:2515:A:N6    | 2.31                     | 0.44              |
| 48:WA:2449:U:H1'  | 48:WA:2746:A:H2    | 1.81                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 48:WA:2564:G:N2    | 48:WA:2567:A:OP2   | 2.36                     | 0.44              |
| 48:WA:2589:A:O2'   | 48:WA:2590:C:O4'   | 2.32                     | 0.44              |
| 48:WA:3672:C:H2'   | 48:WA:3673:G:C8    | 2.53                     | 0.44              |
| 48:WA:3912:C:H2'   | 48:WA:3913:C:C6    | 2.52                     | 0.44              |
| 48:WA:4663:G:N2    | 48:WA:5006:C:O3'   | 2.51                     | 0.44              |
| 51:ZA:1010:G:H2'   | 51:ZA:1011:A:C8    | 2.52                     | 0.44              |
| 51:ZA:1408:U:H2'   | 51:ZA:1409:A:C8    | 2.53                     | 0.44              |
| 59:HB:384:VAL:HG22 | 59:HB:390:ARG:HG2  | 1.99                     | 0.44              |
| 72:UB:46:LYS:HD3   | 72:UB:97:ILE:HG22  | 2.00                     | 0.44              |
| 74:WB:14:ILE:HG22  | 74:WB:25:VAL:HG11  | 1.98                     | 0.44              |
| 74:WB:50:PHE:HB3   | 74:WB:63:VAL:HG13  | 1.98                     | 0.44              |
| 2:B:252:ALA:HB1    | 48:WA:4526:G:C2    | 2.52                     | 0.44              |
| 7:G:158:GLU:OE2    | 7:G:166:ARG:NH2    | 2.34                     | 0.44              |
| 14:N:27:VAL:HG13   | 14:N:98:ALA:HB1    | 1.98                     | 0.44              |
| 14:N:178:ARG:NH1   | 14:N:182:GLU:OE2   | 2.50                     | 0.44              |
| 40:NA:69:ARG:HG3   | 40:NA:82:MET:HE1   | 1.98                     | 0.44              |
| 46:UA:67:G:H2'     | 46:UA:68:G:H8      | 1.82                     | 0.44              |
| 48:WA:955:G:H2'    | 48:WA:956:G:H8     | 1.82                     | 0.44              |
| 48:WA:1405:G:H2'   | 48:WA:1406:G:C8    | 2.52                     | 0.44              |
| 48:WA:1414:G:H2'   | 48:WA:1415:C:C6    | 2.53                     | 0.44              |
| 48:WA:1444:C:N3    | 48:WA:1445:A:N6    | 2.65                     | 0.44              |
| 48:WA:1727:U:H2'   | 48:WA:1728:U:C6    | 2.52                     | 0.44              |
| 48:WA:2612:G:H2'   | 48:WA:2613:A:H8    | 1.83                     | 0.44              |
| 51:ZA:375:U:H2'    | 51:ZA:376:A:C8     | 2.53                     | 0.44              |
| 51:ZA:419:G:N2     | 51:ZA:661:U:O2     | 2.51                     | 0.44              |
| 53:BB:87:ILE:HG22  | 53:BB:101:HIS:HB2  | 2.00                     | 0.44              |
| 68:QB:106:GLN:O    | 68:QB:110:ILE:HG22 | 2.17                     | 0.44              |
| 71:TB:42:HIS:HB3   | 71:TB:93:SER:HB3   | 1.99                     | 0.44              |
| 88:HC:364:HIS:CD2  | 88:HC:421:LEU:HG   | 2.53                     | 0.44              |
| 2:B:384:GLU:OE2    | 22:V:14:TYR:OH     | 2.32                     | 0.44              |
| 24:X:50:ARG:HB2    | 24:X:115:ARG:HH21  | 1.82                     | 0.44              |
| 35:IA:34:CYS:HB3   | 35:IA:39:TYR:H     | 1.82                     | 0.44              |
| 48:WA:6:C:H2'      | 48:WA:7:C:H6       | 1.82                     | 0.44              |
| 48:WA:1819:U:H2'   | 48:WA:1820:G:O4'   | 2.18                     | 0.44              |
| 48:WA:1935:G:H8    | 48:WA:1935:G:O5'   | 2.00                     | 0.44              |
| 51:ZA:65:C:C2      | 58:GB:133:LEU:HD22 | 2.53                     | 0.44              |
| 51:ZA:1376:A:OP1   | 69:RB:67:ARG:NH1   | 2.41                     | 0.44              |
| 51:ZA:1802:C:H2'   | 51:ZA:1803:U:C6    | 2.53                     | 0.44              |
| 10:J:57:VAL:HG12   | 10:J:60:PHE:H      | 1.83                     | 0.44              |
| 25:Y:88:ASP:O      | 25:Y:121:ARG:NH1   | 2.44                     | 0.44              |
| 29:CA:23:ARG:NE    | 29:CA:25:TYR:OH    | 2.36                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 36:JA:12:LEU:HG    | 36:JA:16:ARG:HE    | 1.82                     | 0.44              |
| 37:KA:2:SER:N      | 48:WA:2408:G:N7    | 2.65                     | 0.44              |
| 48:WA:4:G:H2'      | 48:WA:5:A:C8       | 2.52                     | 0.44              |
| 48:WA:169:A:C2     | 48:WA:267:G:C2     | 3.05                     | 0.44              |
| 48:WA:325:U:H2'    | 48:WA:326:C:C6     | 2.52                     | 0.44              |
| 48:WA:2297:C:H2'   | 48:WA:2298:G:C8    | 2.52                     | 0.44              |
| 48:WA:2650:G:H2'   | 48:WA:2651:G:H8    | 1.83                     | 0.44              |
| 48:WA:3738:A:H2'   | 48:WA:3739:A:H8    | 1.83                     | 0.44              |
| 51:ZA:1098:C:H2'   | 51:ZA:1099:G:C8    | 2.52                     | 0.44              |
| 51:ZA:1324:G:O2'   | 51:ZA:1510:G:O2'   | 2.29                     | 0.44              |
| 51:ZA:1858:G:N7    | 66:OB:146:ARG:NH1  | 2.66                     | 0.44              |
| 56:EB:112:HIS:NE2  | 56:EB:237:SER:OG   | 2.45                     | 0.44              |
| 73:VB:73:ALA:HB1   | 73:VB:78:ILE:HB    | 1.99                     | 0.44              |
| 1:A:34:PHE:HE2     | 7:G:94:ILE:HD11    | 1.83                     | 0.44              |
| 2:B:55:HIS:CE1     | 48:WA:4629:U:HO2'  | 2.34                     | 0.44              |
| 5:E:149:PRO:HB2    | 5:E:206:ILE:HG21   | 2.00                     | 0.44              |
| 13:M:120:TRP:HE1   | 13:M:123:GLU:HB3   | 1.82                     | 0.44              |
| 18:R:5:GLY:O       | 18:R:111:ARG:NH2   | 2.50                     | 0.44              |
| 28:BA:50:ASN:OD1   | 28:BA:51:ASN:N     | 2.50                     | 0.44              |
| 30:DA:107:ASN:OD1  | 30:DA:107:ASN:N    | 2.50                     | 0.44              |
| 33:GA:89:ARG:O     | 33:GA:93:ARG:HG2   | 2.17                     | 0.44              |
| 48:WA:254:G:H2'    | 48:WA:255:C:C6     | 2.52                     | 0.44              |
| 51:ZA:1585:U:O2'   | 51:ZA:1587:G:OP2   | 2.31                     | 0.44              |
| 51:ZA:1855:G:OP2   | 66:OB:147:ARG:NH1  | 2.50                     | 0.44              |
| 86:b:69:LEU:HD22   | 86:b:73:PRO:HA     | 1.99                     | 0.44              |
| 6:F:226:PHE:N      | 6:F:232:ALA:O      | 2.46                     | 0.44              |
| 24:X:73:VAL:HG13   | 24:X:80:ILE:HG22   | 2.00                     | 0.44              |
| 48:WA:1820:G:O2'   | 48:WA:1821:G:OP1   | 2.33                     | 0.44              |
| 48:WA:2260:C:H5''  | 48:WA:2261:G:C8    | 2.53                     | 0.44              |
| 48:WA:2760:G:H2'   | 48:WA:2761:G:C8    | 2.53                     | 0.44              |
| 51:ZA:675:U:H2'    | 51:ZA:676:C:H6     | 1.81                     | 0.44              |
| 51:ZA:1096:G:H1    | 51:ZA:1136:U:H3    | 1.66                     | 0.44              |
| 51:ZA:1671:G:H2'   | 51:ZA:1672:U:C6    | 2.53                     | 0.44              |
| 58:GB:32:MET:HB2   | 58:GB:100:CYS:HB2  | 1.99                     | 0.44              |
| 69:RB:132:ARG:H    | 69:RB:132:ARG:HD2  | 1.82                     | 0.44              |
| 84:GC:87:LEU:HD22  | 84:GC:120:ILE:HD11 | 1.98                     | 0.44              |
| 84:GC:259:TRP:HD1  | 84:GC:266:ILE:HA   | 1.82                     | 0.44              |
| 29:CA:122:VAL:HG12 | 29:CA:124:GLU:H    | 1.83                     | 0.44              |
| 48:WA:2287:A:H2'   | 48:WA:2288:G:H8    | 1.83                     | 0.44              |
| 48:WA:3724:G:H2'   | 48:WA:3725:A:C8    | 2.52                     | 0.44              |
| 48:WA:4920:C:H2'   | 48:WA:4921:G:C8    | 2.49                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 49:XA:63:C:H5'     | 49:XA:64:G:H5''    | 1.99                     | 0.44              |
| 51:ZA:1232:U:H2'   | 51:ZA:1233:G:C8    | 2.52                     | 0.44              |
| 51:ZA:1486:A:O3'   | 54:CB:121:ARG:NH2  | 2.51                     | 0.44              |
| 51:ZA:1543:U:P     | 71:TB:62:ARG:HH22  | 2.41                     | 0.44              |
| 51:ZA:1606:G:O2'   | 51:ZA:1632:G:N2    | 2.50                     | 0.44              |
| 54:CB:191:VAL:HG11 | 54:CB:236:PHE:HA   | 1.99                     | 0.44              |
| 86:b:23:ASP:HB2    | 86:b:90:PHE:HB3    | 1.99                     | 0.44              |
| 4:D:166:ALA:HB1    | 4:D:171:LEU:HD12   | 2.00                     | 0.44              |
| 13:M:49:ARG:HH21   | 48:WA:114:G:P      | 2.41                     | 0.44              |
| 15:O:119:PHE:HE1   | 48:WA:397:G:H22    | 1.66                     | 0.44              |
| 24:X:113:LYS:NZ    | 50:YA:84:A:N1      | 2.66                     | 0.44              |
| 25:Y:41:ALA:HB2    | 25:Y:77:TYR:HE1    | 1.83                     | 0.44              |
| 48:WA:712:A:H2'    | 48:WA:713:C:C6     | 2.53                     | 0.44              |
| 48:WA:1266:C:H2'   | 48:WA:1267:G:C8    | 2.53                     | 0.44              |
| 48:WA:1881:C:H2'   | 48:WA:1882:G:O4'   | 2.17                     | 0.44              |
| 48:WA:2001:A:H2'   | 48:WA:2002:G:C5    | 2.53                     | 0.44              |
| 49:XA:77:A:H62     | 49:XA:99:G:H21     | 1.66                     | 0.44              |
| 51:ZA:921:G:C5     | 74:WB:28:ARG:HD3   | 2.53                     | 0.44              |
| 51:ZA:945:U:O2     | 51:ZA:1045:U:O2'   | 2.35                     | 0.44              |
| 51:ZA:1497:G:N7    | 62:KB:25:LYS:NZ    | 2.62                     | 0.44              |
| 64:MB:41:ALA:HA    | 64:MB:45:ARG:HB2   | 1.99                     | 0.44              |
| 78:AC:11:ALA:HB3   | 78:AC:33:ASP:HB2   | 1.99                     | 0.44              |
| 16:P:178:ARG:NH2   | 26:Z:46:ASP:OD1    | 2.50                     | 0.43              |
| 19:S:78:LYS:NZ     | 48:WA:4303:U:OP1   | 2.51                     | 0.43              |
| 32:FA:9:ARG:HG2    | 32:FA:34:TYR:CZ    | 2.53                     | 0.43              |
| 33:GA:66:LYS:NZ    | 50:YA:97:A:OP2     | 2.43                     | 0.43              |
| 44:SA:50:U:O4      | 44:SA:64:G:O6      | 2.35                     | 0.43              |
| 48:WA:162:A:H2'    | 48:WA:163:A:C8     | 2.53                     | 0.43              |
| 48:WA:460:C:H2'    | 48:WA:461:G:H8     | 1.83                     | 0.43              |
| 48:WA:470:A:H62    | 48:WA:685:G:N2     | 2.16                     | 0.43              |
| 48:WA:1808:G:H2'   | 48:WA:1809:C:C6    | 2.53                     | 0.43              |
| 48:WA:2850:G:O2'   | 48:WA:3840:U:O4    | 2.32                     | 0.43              |
| 48:WA:4461:U:H2'   | 48:WA:4462:U:C6    | 2.53                     | 0.43              |
| 51:ZA:1688:C:H2'   | 51:ZA:1689:C:H6    | 1.83                     | 0.43              |
| 56:EB:204:SER:OG   | 56:EB:205:PHE:N    | 2.51                     | 0.43              |
| 75:XB:94:ILE:HG12  | 75:XB:125:VAL:HG21 | 1.99                     | 0.43              |
| 77:ZB:79:ILE:HB    | 77:ZB:83:LEU:HD23  | 2.00                     | 0.43              |
| 81:DC:33:LYS:HE2   | 81:DC:34:TYR:CZ    | 2.53                     | 0.43              |
| 2:B:92:TYR:HB2     | 2:B:159:VAL:HB     | 1.99                     | 0.43              |
| 8:H:66:GLU:O       | 8:H:69:THR:OG1     | 2.34                     | 0.43              |
| 12:L:12:VAL:O      | 12:L:58:THR:OG1    | 2.24                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:W:135:LYS:NZ   | 48:WA:2438:U:OP2  | 2.51                     | 0.43              |
| 48:WA:408:A:O2'   | 48:WA:411:G:OP2   | 2.26                     | 0.43              |
| 48:WA:1249:U:O4   | 48:WA:1268:G:O6   | 2.36                     | 0.43              |
| 48:WA:3875:G:H2'  | 48:WA:3876:G:C8   | 2.53                     | 0.43              |
| 48:WA:4682:G:H2'  | 48:WA:4683:A:C8   | 2.52                     | 0.43              |
| 50:YA:110:U:O2'   | 50:YA:111:U:O4'   | 2.36                     | 0.43              |
| 54:CB:199:PRO:O   | 54:CB:202:THR:OG1 | 2.35                     | 0.43              |
| 56:EB:45:ILE:HA   | 56:EB:61:VAL:HG11 | 2.01                     | 0.43              |
| 62:KB:1:MET:HG3   | 62:KB:47:LYS:HG3  | 2.00                     | 0.43              |
| 64:MB:79:VAL:HG21 | 64:MB:85:LEU:HD13 | 2.01                     | 0.43              |
| 66:OB:54:CYS:HB2  | 66:OB:84:ARG:HG2  | 1.99                     | 0.43              |
| 76:YB:110:ARG:NH1 | 76:YB:126:GLY:O   | 2.51                     | 0.43              |
| 84:GC:38:LYS:NZ   | 84:GC:63:SER:O    | 2.51                     | 0.43              |
| 87:c:250:PHE:HA   | 87:c:253:PHE:HD2  | 1.82                     | 0.43              |
| 6:F:240:ASN:O     | 6:F:244:ARG:HG2   | 2.18                     | 0.43              |
| 13:M:38:ARG:NH2   | 50:YA:142:U:OP1   | 2.46                     | 0.43              |
| 17:Q:102:LEU:HD22 | 17:Q:138:LEU:HD22 | 2.00                     | 0.43              |
| 23:W:52:LEU:HD22  | 23:W:54:LEU:HD12  | 2.00                     | 0.43              |
| 35:IA:76:HIS:NE2  | 50:YA:93:C:OP1    | 2.43                     | 0.43              |
| 44:SA:25:C:H2'    | 44:SA:26:A:H8     | 1.84                     | 0.43              |
| 48:WA:129:C:H2'   | 48:WA:130:C:C6    | 2.52                     | 0.43              |
| 48:WA:1256:A:N1   | 48:WA:1261:G:O6   | 2.51                     | 0.43              |
| 48:WA:1311:C:H2'  | 48:WA:1312:C:C6   | 2.53                     | 0.43              |
| 48:WA:1685:U:H2'  | 48:WA:1686:A:C8   | 2.53                     | 0.43              |
| 48:WA:2609:C:H2'  | 48:WA:2610:G:C8   | 2.53                     | 0.43              |
| 48:WA:3870:G:H22  | 48:WA:3902:G:H1'  | 1.84                     | 0.43              |
| 48:WA:5032:U:H2'  | 48:WA:5033:G:H8   | 1.84                     | 0.43              |
| 51:ZA:15:U:H2'    | 51:ZA:16:G:O4'    | 2.17                     | 0.43              |
| 51:ZA:219:U:H2'   | 51:ZA:220:U:C6    | 2.53                     | 0.43              |
| 51:ZA:996:A:H2'   | 51:ZA:997:A:C8    | 2.53                     | 0.43              |
| 51:ZA:1648:G:H22  | 51:ZA:1675:A:P    | 2.40                     | 0.43              |
| 6:F:189:LEU:HD21  | 6:F:207:LEU:HD21  | 2.00                     | 0.43              |
| 7:G:139:VAL:HG11  | 7:G:238:LYS:HG3   | 2.01                     | 0.43              |
| 8:H:172:ILE:HD11  | 38:LA:98:LYS:HZ1  | 1.84                     | 0.43              |
| 12:L:34:ASN:ND2   | 48:WA:1926:C:OP1  | 2.51                     | 0.43              |
| 13:M:193:ARG:O    | 13:M:197:THR:OG1  | 2.27                     | 0.43              |
| 19:S:4:THR:OG1    | 48:WA:4210:U:OP2  | 2.29                     | 0.43              |
| 33:GA:52:LYS:NZ   | 50:YA:63:U:O2'    | 2.36                     | 0.43              |
| 35:IA:12:ARG:O    | 48:WA:2406:A:O2'  | 2.32                     | 0.43              |
| 43:RA:66:ASN:OD1  | 43:RA:66:ASN:N    | 2.51                     | 0.43              |
| 48:WA:229:G:H2'   | 48:WA:230:G:H8    | 1.83                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 48:WA:1690:G:H2'   | 48:WA:1691:G:C8    | 2.53                     | 0.43              |
| 48:WA:2000:A:O2'   | 48:WA:2001:A:O4'   | 2.31                     | 0.43              |
| 48:WA:2000:A:H1'   | 48:WA:2021:C:O2'   | 2.18                     | 0.43              |
| 48:WA:4910:G:H1'   | 48:WA:4915:G:H22   | 1.83                     | 0.43              |
| 51:ZA:547:G:H2'    | 51:ZA:549:C:C6     | 2.53                     | 0.43              |
| 51:ZA:1503:C:H2'   | 51:ZA:1504:U:C6    | 2.53                     | 0.43              |
| 57:FB:176:GLU:OE2  | 57:FB:187:SER:OG   | 2.36                     | 0.43              |
| 84:GC:163:PRO:HB2  | 84:GC:179:LEU:HB3  | 2.00                     | 0.43              |
| 88:HC:250:LEU:HD22 | 88:HC:324:ASN:HB2  | 2.00                     | 0.43              |
| 1:A:14:SER:OG      | 48:WA:1630:C:OP1   | 2.36                     | 0.43              |
| 2:B:298:LEU:HD13   | 2:B:300:LYS:HE3    | 2.00                     | 0.43              |
| 3:C:221:PHE:HB3    | 3:C:227:ILE:HG21   | 1.99                     | 0.43              |
| 13:M:93:LYS:NZ     | 48:WA:4179:C:OP1   | 2.38                     | 0.43              |
| 16:P:67:ILE:HD13   | 16:P:98:LEU:HD11   | 2.01                     | 0.43              |
| 18:R:16:CYS:SG     | 18:R:17:LEU:N      | 2.92                     | 0.43              |
| 21:U:107:ASN:HD21  | 21:U:111:GLU:HB2   | 1.83                     | 0.43              |
| 24:X:59:ARG:HD2    | 48:WA:209:U:H5'    | 1.99                     | 0.43              |
| 34:HA:31:GLY:HA3   | 48:WA:310:G:C4     | 2.53                     | 0.43              |
| 40:NA:77:CYS:SG    | 40:NA:79:SER:OG    | 2.65                     | 0.43              |
| 43:RA:147:HIS:CD2  | 43:RA:148:PRO:HD3  | 2.53                     | 0.43              |
| 45:TA:69:G:H2'     | 45:TA:70:G:H8      | 1.84                     | 0.43              |
| 48:WA:474:C:H2'    | 48:WA:475:G:C8     | 2.53                     | 0.43              |
| 48:WA:1678:C:N4    | 48:WA:4380:A:H2'   | 2.33                     | 0.43              |
| 48:WA:1781:U:H2'   | 48:WA:1782:A:C8    | 2.54                     | 0.43              |
| 48:WA:2641:U:H2'   | 48:WA:2696:G:C6    | 2.53                     | 0.43              |
| 48:WA:4188:A:H2'   | 48:WA:4189:G:H8    | 1.83                     | 0.43              |
| 48:WA:4580:G:H2'   | 48:WA:4581:U:C6    | 2.53                     | 0.43              |
| 50:YA:57:C:O2      | 50:YA:61:A:O2'     | 2.36                     | 0.43              |
| 51:ZA:70:G:H21     | 51:ZA:79:A:H62     | 1.65                     | 0.43              |
| 51:ZA:1513:C:H2'   | 51:ZA:1514:G:C8    | 2.52                     | 0.43              |
| 57:FB:40:ALA:HB1   | 57:FB:45:TYR:CD1   | 2.54                     | 0.43              |
| 63:LB:12:LYS:HA    | 63:LB:56:ILE:HD13  | 1.99                     | 0.43              |
| 67:PB:41:GLN:HG3   | 67:PB:84:ILE:HD13  | 2.00                     | 0.43              |
| 68:QB:122:TYR:HA   | 68:QB:126:VAL:HG23 | 1.99                     | 0.43              |
| 70:SB:33:ILE:HD13  | 70:SB:71:MET:HE1   | 2.01                     | 0.43              |
| 78:AC:44:ILE:HG21  | 78:AC:65:PRO:HG2   | 2.00                     | 0.43              |
| 88:HC:372:PHE:HE1  | 88:HC:402:VAL:HG21 | 1.83                     | 0.43              |
| 2:B:55:HIS:CD2     | 48:WA:4629:U:HO2'  | 2.36                     | 0.43              |
| 2:B:100:ARG:NE     | 48:WA:4913:A:OP2   | 2.52                     | 0.43              |
| 2:B:317:LEU:HB3    | 48:WA:5003:U:H4'   | 2.00                     | 0.43              |
| 18:R:111:ARG:NH2   | 48:WA:2064:C:O2'   | 2.52                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 20:T:29:VAL:HG21   | 20:T:68:SER:HB2    | 2.01                     | 0.43              |
| 27:AA:47:LYS:NZ    | 48:WA:1466:C:O3'   | 2.50                     | 0.43              |
| 29:CA:68:LEU:HA    | 29:CA:108:TYR:HB2  | 2.01                     | 0.43              |
| 38:LA:80:ARG:HH21  | 48:WA:4698:C:H4'   | 1.82                     | 0.43              |
| 45:TA:23:A:H2'     | 45:TA:24:G:H8      | 1.84                     | 0.43              |
| 48:WA:1087:C:H2'   | 48:WA:1088:C:C6    | 2.54                     | 0.43              |
| 48:WA:1474:C:H2'   | 48:WA:1475:U:C6    | 2.54                     | 0.43              |
| 48:WA:1755:G:H2'   | 48:WA:1756:U:C2    | 2.53                     | 0.43              |
| 48:WA:2027:A:H8    | 48:WA:2028:A:H1'   | 1.83                     | 0.43              |
| 48:WA:3666:G:H2'   | 48:WA:3667:G:C8    | 2.52                     | 0.43              |
| 48:WA:3713:A:O2'   | 48:WA:3715:U:OP2   | 2.27                     | 0.43              |
| 48:WA:3729:A:H2'   | 48:WA:3730:A:C8    | 2.54                     | 0.43              |
| 51:ZA:1230:C:H2'   | 51:ZA:1231:C:H6    | 1.83                     | 0.43              |
| 51:ZA:1386:A:OP2   | 55:DB:198:SER:OG   | 2.33                     | 0.43              |
| 51:ZA:1419:C:H4'   | 51:ZA:1420:G:C2    | 2.54                     | 0.43              |
| 51:ZA:1461:G:O2'   | 51:ZA:1465:A:N6    | 2.51                     | 0.43              |
| 51:ZA:1576:G:H2'   | 51:ZA:1577:G:C8    | 2.54                     | 0.43              |
| 56:EB:179:ASN:HD22 | 56:EB:230:LYS:HA   | 1.82                     | 0.43              |
| 60:IB:62:VAL:HG12  | 60:IB:77:ARG:HA    | 2.01                     | 0.43              |
| 62:KB:51:SER:O     | 62:KB:55:ARG:HG2   | 2.18                     | 0.43              |
| 69:RB:73:LEU:O     | 69:RB:76:GLU:HG3   | 2.17                     | 0.43              |
| 84:GC:8:ARG:HB3    | 84:GC:309:VAL:HG23 | 2.00                     | 0.43              |
| 2:B:28:LYS:NZ      | 48:WA:4584:C:OP2   | 2.49                     | 0.43              |
| 2:B:31:SER:OG      | 48:WA:4716:C:OP1   | 2.31                     | 0.43              |
| 4:D:176:SER:HB3    | 48:WA:4325:A:H4'   | 2.00                     | 0.43              |
| 6:F:154:TYR:OH     | 6:F:187:GLU:OE2    | 2.36                     | 0.43              |
| 10:J:112:HIS:HD1   | 10:J:126:TYR:H     | 1.67                     | 0.43              |
| 12:L:72:TYR:HD1    | 12:L:75:LYS:HE2    | 1.82                     | 0.43              |
| 26:Z:117:LEU:HB3   | 26:Z:140:VAL:HG21  | 2.01                     | 0.43              |
| 48:WA:2732:U:H2'   | 48:WA:2733:C:C6    | 2.54                     | 0.43              |
| 51:ZA:24:C:O2'     | 51:ZA:25:A:OP1     | 2.35                     | 0.43              |
| 51:ZA:193:C:H2'    | 51:ZA:194:C:H6     | 1.84                     | 0.43              |
| 51:ZA:943:U:H2'    | 51:ZA:944:A:H8     | 1.83                     | 0.43              |
| 51:ZA:1144:A:H2'   | 51:ZA:1145:A:C8    | 2.54                     | 0.43              |
| 72:UB:46:LYS:HD2   | 72:UB:101:ILE:HD13 | 2.01                     | 0.43              |
| 82:EC:84:LYS:HE3   | 82:EC:84:LYS:HB3   | 1.90                     | 0.43              |
| 13:M:54:LYS:NZ     | 48:WA:153:G:OP2    | 2.47                     | 0.43              |
| 15:O:140:SER:OG    | 15:O:182:LYS:O     | 2.25                     | 0.43              |
| 25:Y:22:LYS:NZ     | 25:Y:129:TRP:O     | 2.50                     | 0.43              |
| 27:AA:18:ARG:NH1   | 48:WA:1670:A:O3'   | 2.44                     | 0.43              |
| 48:WA:1506:G:H2'   | 48:WA:1507:C:C6    | 2.53                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 48:WA:2626:G:H2'   | 48:WA:2627:U:H6    | 1.82                     | 0.43              |
| 48:WA:3857:C:H2'   | 48:WA:3858:A:H8    | 1.83                     | 0.43              |
| 50:YA:102:G:OP2    | 50:YA:104:A:O2'    | 2.27                     | 0.43              |
| 51:ZA:202:G:H2'    | 51:ZA:203:G:C8     | 2.54                     | 0.43              |
| 51:ZA:388:U:H2'    | 51:ZA:389:A:C8     | 2.54                     | 0.43              |
| 51:ZA:1016:U:OP2   | 79:BC:20:LYS:NZ    | 2.52                     | 0.43              |
| 51:ZA:1103:C:H2'   | 51:ZA:1104:G:H8    | 1.84                     | 0.43              |
| 61:JB:111:GLN:HE21 | 61:JB:123:ILE:HG22 | 1.83                     | 0.43              |
| 65:NB:3:ARG:HB2    | 65:NB:6:ALA:HB3    | 2.01                     | 0.43              |
| 74:WB:113:HIS:NE2  | 74:WB:114:GLU:OE2  | 2.51                     | 0.43              |
| 80:CC:33:GLU:HG2   | 80:CC:41:SER:HB3   | 2.01                     | 0.43              |
| 88:HC:273:LYS:NZ   | 88:HC:300:SER:O    | 2.51                     | 0.43              |
| 3:C:278:ASN:OD1    | 3:C:279:LEU:N      | 2.52                     | 0.43              |
| 4:D:69:ILE:HG12    | 19:S:31:MET:HG3    | 2.01                     | 0.43              |
| 5:E:48:ARG:HG2     | 48:WA:986:U:OP1    | 2.19                     | 0.43              |
| 6:F:181:TYR:CZ     | 6:F:202:GLU:HG2    | 2.54                     | 0.43              |
| 16:P:75:ARG:HA     | 16:P:78:LYS:HD3    | 2.00                     | 0.43              |
| 20:T:80:LYS:HG2    | 20:T:110:TYR:CE2   | 2.54                     | 0.43              |
| 27:AA:10:HIS:NE2   | 48:WA:1879:G:O6    | 2.44                     | 0.43              |
| 48:WA:4451:A:H8    | 92:WA:5228:ANM:H61 | 1.83                     | 0.43              |
| 48:WA:4637:A:O2'   | 48:WA:4639:G:OP1   | 2.31                     | 0.43              |
| 48:WA:4718:C:H2'   | 48:WA:4719:A:C8    | 2.52                     | 0.43              |
| 48:WA:4962:G:H2'   | 48:WA:4963:G:C8    | 2.52                     | 0.43              |
| 50:YA:66:A:H2'     | 50:YA:67:U:C6      | 2.54                     | 0.43              |
| 51:ZA:12:U:H2'     | 51:ZA:13:C:H6      | 1.84                     | 0.43              |
| 51:ZA:14:C:H2'     | 51:ZA:15:U:C6      | 2.53                     | 0.43              |
| 51:ZA:929:G:H2'    | 51:ZA:930:C:O4'    | 2.18                     | 0.43              |
| 51:ZA:1563:G:H5''  | 71:TB:121:ARG:NH1  | 2.34                     | 0.43              |
| 51:ZA:1654:G:H2'   | 51:ZA:1655:C:C6    | 2.54                     | 0.43              |
| 76:YB:83:LYS:HD2   | 76:YB:91:LEU:HD22  | 2.01                     | 0.43              |
| 1:A:230:PRO:HG2    | 1:A:233:ARG:HB3    | 2.01                     | 0.43              |
| 12:L:86:TRP:O      | 12:L:89:THR:OG1    | 2.35                     | 0.43              |
| 30:DA:65:LYS:O     | 30:DA:75:ARG:NH2   | 2.49                     | 0.43              |
| 48:WA:971:A:H5'    | 48:WA:972:C:H2'    | 2.00                     | 0.43              |
| 48:WA:1881:C:O2'   | 48:WA:1893:A:N3    | 2.48                     | 0.43              |
| 48:WA:2376:A:H2'   | 48:WA:2377:A:C8    | 2.54                     | 0.43              |
| 48:WA:3863:A:H2'   | 48:WA:3864:A:C8    | 2.52                     | 0.43              |
| 48:WA:4239:C:OP1   | 48:WA:4329:C:O2'   | 2.31                     | 0.43              |
| 48:WA:4568:U:H2'   | 48:WA:4569:G:O4'   | 2.19                     | 0.43              |
| 51:ZA:12:U:H2'     | 51:ZA:13:C:C6      | 2.54                     | 0.43              |
| 51:ZA:479:C:H4'    | 88:HC:255:LYS:HD2  | 2.01                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 51:ZA:959:G:H1'   | 51:ZA:964:A:H61    | 1.83                     | 0.43              |
| 51:ZA:1407:U:H2'  | 51:ZA:1408:U:C6    | 2.54                     | 0.43              |
| 58:GB:21:GLU:O    | 58:GB:25:ARG:HG3   | 2.19                     | 0.43              |
| 64:MB:52:LEU:HD11 | 64:MB:78:LYS:HE3   | 2.00                     | 0.43              |
| 76:YB:62:THR:HA   | 76:YB:69:THR:HG22  | 2.01                     | 0.43              |
| 76:YB:100:LYS:HE2 | 76:YB:107:ARG:HH21 | 1.84                     | 0.43              |
| 29:CA:53:ALA:HA   | 29:CA:88:LEU:HD21  | 2.01                     | 0.42              |
| 29:CA:57:MET:HG2  | 29:CA:88:LEU:HD23  | 2.01                     | 0.42              |
| 37:KA:36:ARG:NH2  | 48:WA:413:G:O4'    | 2.53                     | 0.42              |
| 48:WA:281:U:H2'   | 48:WA:282:C:H6     | 1.83                     | 0.42              |
| 48:WA:1302:G:H2'  | 48:WA:1303:C:C6    | 2.54                     | 0.42              |
| 48:WA:1664:C:H2'  | 48:WA:1665:C:H6    | 1.83                     | 0.42              |
| 48:WA:1939:C:OP2  | 48:WA:1940:C:O2'   | 2.25                     | 0.42              |
| 48:WA:2092:U:OP1  | 48:WA:2268:C:N4    | 2.52                     | 0.42              |
| 48:WA:2665:G:N2   | 48:WA:2678:A:O2'   | 2.52                     | 0.42              |
| 48:WA:2899:G:H2'  | 48:WA:2900:G:C8    | 2.51                     | 0.42              |
| 48:WA:3709:U:H2'  | 48:WA:3710:C:C6    | 2.54                     | 0.42              |
| 48:WA:4993:U:H2'  | 48:WA:4994:G:C8    | 2.53                     | 0.42              |
| 49:XA:4:U:H2'     | 49:XA:5:A:C8       | 2.54                     | 0.42              |
| 50:YA:5:U:H2'     | 50:YA:6:C:H6       | 1.84                     | 0.42              |
| 50:YA:153:C:H2'   | 50:YA:154:G:H8     | 1.84                     | 0.42              |
| 51:ZA:1809:A:H2'  | 51:ZA:1810:U:C6    | 2.54                     | 0.42              |
| 62:KB:1:MET:HE1   | 62:KB:44:HIS:CE1   | 2.54                     | 0.42              |
| 84:GC:2:THR:O     | 84:GC:2:THR:OG1    | 2.34                     | 0.42              |
| 3:C:163:LYS:HB2   | 3:C:166:GLU:HG3    | 2.01                     | 0.42              |
| 12:L:118:MET:HE1  | 48:WA:4930:C:O2    | 2.19                     | 0.42              |
| 16:P:150:ARG:NH2  | 48:WA:1501:C:OP1   | 2.52                     | 0.42              |
| 22:V:112:ALA:O    | 22:V:116:LYS:HG2   | 2.20                     | 0.42              |
| 48:WA:190:G:H2'   | 48:WA:191:G:H8     | 1.83                     | 0.42              |
| 48:WA:2083:C:H2'  | 48:WA:2084:G:C8    | 2.53                     | 0.42              |
| 48:WA:4156:G:H2'  | 48:WA:4157:C:C6    | 2.54                     | 0.42              |
| 48:WA:4639:G:H2'  | 48:WA:4640:U:C6    | 2.54                     | 0.42              |
| 51:ZA:479:C:H2'   | 51:ZA:480:G:C8     | 2.54                     | 0.42              |
| 51:ZA:1079:C:O2'  | 51:ZA:1182:A:N1    | 2.49                     | 0.42              |
| 51:ZA:1232:U:H2'  | 51:ZA:1233:G:H8    | 1.84                     | 0.42              |
| 51:ZA:1294:G:H2'  | 51:ZA:1295:A:H8    | 1.83                     | 0.42              |
| 51:ZA:1318:G:H2'  | 51:ZA:1319:U:C6    | 2.54                     | 0.42              |
| 51:ZA:1671:G:H2'  | 51:ZA:1672:U:H6    | 1.83                     | 0.42              |
| 51:ZA:1780:G:H2'  | 51:ZA:1781:A:C8    | 2.54                     | 0.42              |
| 51:ZA:1842:C:H2'  | 51:ZA:1843:G:C8    | 2.54                     | 0.42              |
| 74:WB:55:ASP:OD1  | 74:WB:56:HIS:N     | 2.48                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 80:CC:36:ASP:OD1   | 80:CC:36:ASP:N     | 2.52                     | 0.42              |
| 1:A:21:LYS:HE3     | 48:WA:2745:A:H1'   | 2.00                     | 0.42              |
| 6:F:148:SER:OG     | 6:F:244:ARG:NH2    | 2.49                     | 0.42              |
| 10:J:24:ILE:HG12   | 10:J:128:LEU:HB3   | 2.00                     | 0.42              |
| 16:P:39:THR:OG1    | 16:P:44:ASN:ND2    | 2.47                     | 0.42              |
| 33:GA:109:ARG:HH22 | 48:WA:267:G:P      | 2.42                     | 0.42              |
| 35:IA:44:LYS:N     | 48:WA:22:G:OP1     | 2.40                     | 0.42              |
| 44:SA:26:A:H61     | 44:SA:44:A:H61     | 1.66                     | 0.42              |
| 48:WA:727:G:H2'    | 48:WA:728:C:C6     | 2.54                     | 0.42              |
| 48:WA:741:G:H2'    | 48:WA:742:G:H8     | 1.85                     | 0.42              |
| 48:WA:1492:G:H2'   | 48:WA:1493:A:C8    | 2.53                     | 0.42              |
| 48:WA:1647:C:H2'   | 48:WA:1648:A:C8    | 2.53                     | 0.42              |
| 48:WA:2391:A:H2'   | 48:WA:2392:G:C8    | 2.54                     | 0.42              |
| 48:WA:2448:C:H2'   | 48:WA:2449:U:C6    | 2.53                     | 0.42              |
| 48:WA:4387:A:H61   | 48:WA:4533:U:H5'   | 1.83                     | 0.42              |
| 51:ZA:920:A:O2'    | 51:ZA:922:A:O5'    | 2.37                     | 0.42              |
| 51:ZA:1093:A:H2'   | 51:ZA:1094:C:H6    | 1.84                     | 0.42              |
| 51:ZA:1112:U:H2'   | 51:ZA:1113:A:C8    | 2.54                     | 0.42              |
| 51:ZA:1199:A:H2'   | 51:ZA:1200:A:C8    | 2.54                     | 0.42              |
| 51:ZA:1488:C:H3'   | 51:ZA:1489:A:H4'   | 2.00                     | 0.42              |
| 58:GB:2:LYS:HB2    | 58:GB:108:VAL:HG22 | 2.00                     | 0.42              |
| 75:XB:46:HIS:HB3   | 75:XB:101:LEU:HD11 | 2.01                     | 0.42              |
| 2:B:55:HIS:HB2     | 2:B:369:ASP:HB2    | 2.01                     | 0.42              |
| 9:I:35:ASP:HA      | 9:I:87:ILE:O       | 2.19                     | 0.42              |
| 10:J:87:LEU:HD13   | 10:J:87:LEU:HA     | 1.88                     | 0.42              |
| 14:N:34:VAL:HG22   | 14:N:103:LYS:HB3   | 2.02                     | 0.42              |
| 14:N:68:ARG:NH2    | 48:WA:4566:A:OP1   | 2.52                     | 0.42              |
| 33:GA:97:LYS:HD3   | 48:WA:135:G:C6     | 2.55                     | 0.42              |
| 37:KA:15:LYS:HD3   | 50:YA:45:C:P       | 2.59                     | 0.42              |
| 48:WA:66:A:O2'     | 48:WA:326:C:O2     | 2.33                     | 0.42              |
| 48:WA:478:G:H2'    | 48:WA:479:G:C8     | 2.54                     | 0.42              |
| 48:WA:1346:C:H2'   | 48:WA:1347:A:C8    | 2.54                     | 0.42              |
| 48:WA:2000:A:H4'   | 86:b:9:TRP:HZ2     | 1.85                     | 0.42              |
| 48:WA:2628:U:H1'   | 48:WA:2631:C:H41   | 1.84                     | 0.42              |
| 48:WA:2642:G:H2'   | 48:WA:2643:A:C8    | 2.55                     | 0.42              |
| 51:ZA:409:C:H2'    | 51:ZA:410:G:C8     | 2.54                     | 0.42              |
| 51:ZA:536:A:H61    | 51:ZA:549:C:N4     | 2.17                     | 0.42              |
| 62:KB:15:LEU:HD13  | 62:KB:21:MET:HB2   | 2.01                     | 0.42              |
| 70:SB:89:ASP:OD1   | 70:SB:89:ASP:N     | 2.50                     | 0.42              |
| 1:A:242:ARG:NH2    | 1:A:243:THR:O      | 2.52                     | 0.42              |
| 3:C:350:ARG:HD2    | 48:WA:725:C:OP1    | 2.19                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:J:13:ARG:O     | 10:J:136:ARG:NH1  | 2.52                     | 0.42              |
| 12:L:96:GLU:OE2   | 12:L:100:ARG:NH2  | 2.52                     | 0.42              |
| 19:S:87:LYS:HZ2   | 48:WA:4307:G:N2   | 2.17                     | 0.42              |
| 23:W:88:LYS:HA    | 23:W:91:GLU:HG2   | 2.02                     | 0.42              |
| 29:CA:39:LYS:HE3  | 48:WA:2372:A:H5'  | 2.01                     | 0.42              |
| 48:WA:32:G:H21    | 48:WA:50:C:H5     | 1.66                     | 0.42              |
| 48:WA:655:C:H2'   | 48:WA:656:C:C6    | 2.55                     | 0.42              |
| 48:WA:912:G:H2'   | 48:WA:913:U:H6    | 1.84                     | 0.42              |
| 48:WA:1463:C:H2'  | 48:WA:1464:A:H8   | 1.84                     | 0.42              |
| 48:WA:1463:C:H2'  | 48:WA:1464:A:C8   | 2.54                     | 0.42              |
| 48:WA:2001:A:H2'  | 48:WA:2002:G:C4   | 2.55                     | 0.42              |
| 48:WA:2680:A:H2'  | 48:WA:2681:G:H8   | 1.85                     | 0.42              |
| 48:WA:3872:C:H2'  | 48:WA:3873:A:C8   | 2.54                     | 0.42              |
| 51:ZA:1171:G:O2'  | 51:ZA:1187:G:O6   | 2.38                     | 0.42              |
| 51:ZA:1577:G:O2'  | 51:ZA:1579:A:N3   | 2.51                     | 0.42              |
| 51:ZA:1736:G:H2'  | 51:ZA:1737:G:C8   | 2.55                     | 0.42              |
| 61:JB:101:LYS:N   | 61:JB:104:ASP:OD2 | 2.47                     | 0.42              |
| 62:KB:6:LYS:HE3   | 62:KB:6:LYS:HB3   | 1.83                     | 0.42              |
| 70:SB:120:HIS:CE1 | 70:SB:124:ARG:HD2 | 2.54                     | 0.42              |
| 80:CC:23:SER:OG   | 80:CC:24:GLN:OE1  | 2.31                     | 0.42              |
| 1:A:54:ARG:HG2    | 1:A:56:ALA:H      | 1.85                     | 0.42              |
| 2:B:116:ARG:NH2   | 48:WA:4989:C:OP1  | 2.52                     | 0.42              |
| 5:E:45:HIS:ND1    | 5:E:46:CYS:O      | 2.50                     | 0.42              |
| 9:I:86:HIS:HB3    | 9:I:139:ARG:HG2   | 2.02                     | 0.42              |
| 11:K:130:LYS:HE3  | 11:K:132:SER:HB2  | 2.00                     | 0.42              |
| 33:GA:34:ALA:HA   | 33:GA:37:THR:HG22 | 2.01                     | 0.42              |
| 46:UA:43:A:H3'    | 46:UA:44:A:C8     | 2.54                     | 0.42              |
| 48:WA:1300:C:H2'  | 48:WA:1301:G:H8   | 1.85                     | 0.42              |
| 48:WA:2081:G:H2'  | 48:WA:2082:U:H6   | 1.84                     | 0.42              |
| 48:WA:2295:U:H2'  | 48:WA:2296:G:C8   | 2.55                     | 0.42              |
| 51:ZA:495:U:O2'   | 56:EB:27:PHE:O    | 2.34                     | 0.42              |
| 51:ZA:681:U:H4'   | 75:XB:9:THR:HG22  | 2.00                     | 0.42              |
| 51:ZA:694:G:H22   | 51:ZA:732:U:H3    | 1.67                     | 0.42              |
| 51:ZA:1383:A:H4'  | 55:DB:194:LEU:HG  | 2.01                     | 0.42              |
| 58:GB:148:SER:N   | 58:GB:151:ASP:OD2 | 2.52                     | 0.42              |
| 84:GC:104:HIS:NE2 | 84:GC:122:SER:OG  | 2.50                     | 0.42              |
| 1:A:28:ARG:HE     | 1:A:123:ARG:HD3   | 1.84                     | 0.42              |
| 1:A:179:ILE:O     | 48:WA:3655:A:O2'  | 2.19                     | 0.42              |
| 2:B:2:SER:N       | 48:WA:4522:G:H5'  | 2.34                     | 0.42              |
| 4:D:12:TYR:OH     | 48:WA:4267:U:OP1  | 2.38                     | 0.42              |
| 17:Q:108:ARG:NH1  | 48:WA:2901:C:OP2  | 2.41                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 19:S:75:VAL:HG22   | 19:S:88:ARG:HG2    | 2.01                     | 0.42              |
| 22:V:49:ILE:O      | 22:V:52:THR:OG1    | 2.29                     | 0.42              |
| 25:Y:79:HIS:ND1    | 48:WA:2582:U:O2'   | 2.43                     | 0.42              |
| 30:DA:67:LYS:HG2   | 30:DA:68:HIS:CD2   | 2.55                     | 0.42              |
| 33:GA:96:ASN:N     | 33:GA:96:ASN:OD1   | 2.50                     | 0.42              |
| 48:WA:325:U:H2'    | 48:WA:326:C:H6     | 1.84                     | 0.42              |
| 48:WA:1263:G:H2'   | 48:WA:1264:G:H8    | 1.85                     | 0.42              |
| 48:WA:1513:U:H2'   | 48:WA:1514:G:H8    | 1.85                     | 0.42              |
| 48:WA:2545:A:H5'   | 50:YA:127:U:H1'    | 2.02                     | 0.42              |
| 48:WA:2734:G:H2'   | 48:WA:2735:C:C6    | 2.55                     | 0.42              |
| 48:WA:3935:G:H2'   | 48:WA:3936:G:H8    | 1.84                     | 0.42              |
| 48:WA:4131:G:O6    | 48:WA:4158:G:N2    | 2.53                     | 0.42              |
| 48:WA:4194:A:H2'   | 48:WA:4195:C:C6    | 2.55                     | 0.42              |
| 48:WA:4565:U:C2    | 48:WA:4566:A:C8    | 3.08                     | 0.42              |
| 48:WA:4956:G:H2'   | 48:WA:4957:A:C8    | 2.52                     | 0.42              |
| 51:ZA:161:U:O2'    | 58:GB:87:ARG:NH1   | 2.53                     | 0.42              |
| 51:ZA:674:C:H2'    | 51:ZA:675:U:C6     | 2.55                     | 0.42              |
| 51:ZA:909:G:H2'    | 51:ZA:910:G:H8     | 1.84                     | 0.42              |
| 53:BB:43:ASN:OD1   | 53:BB:43:ASN:N     | 2.52                     | 0.42              |
| 64:MB:79:VAL:HG11  | 64:MB:85:LEU:HB2   | 2.01                     | 0.42              |
| 66:OB:126:ILE:N    | 78:AC:56:ALA:O     | 2.51                     | 0.42              |
| 84:GC:152:SER:N    | 84:GC:168:CYS:O    | 2.52                     | 0.42              |
| 1:A:83:HIS:HB3     | 41:OA:64:VAL:HG13  | 2.01                     | 0.42              |
| 2:B:82:PRO:HG3     | 2:B:171:LEU:HD21   | 2.02                     | 0.42              |
| 27:AA:18:ARG:HH12  | 48:WA:1671:A:P     | 2.43                     | 0.42              |
| 48:WA:1192:U:H2'   | 48:WA:1193:G:N3    | 2.34                     | 0.42              |
| 48:WA:1246:G:H2'   | 48:WA:1247:C:C6    | 2.55                     | 0.42              |
| 48:WA:1348:C:H2'   | 48:WA:1349:G:C8    | 2.54                     | 0.42              |
| 48:WA:1788:A:H2'   | 48:WA:1791:C:C5    | 2.55                     | 0.42              |
| 48:WA:2495:G:O2'   | 50:YA:127:U:OP1    | 2.29                     | 0.42              |
| 48:WA:2664:G:H2'   | 48:WA:2665:G:C8    | 2.55                     | 0.42              |
| 48:WA:2737:G:H2'   | 48:WA:2738:G:C8    | 2.53                     | 0.42              |
| 50:YA:141:C:H2'    | 50:YA:142:U:C6     | 2.55                     | 0.42              |
| 51:ZA:323:C:N4     | 51:ZA:328:U:OP1    | 2.37                     | 0.42              |
| 51:ZA:1803:U:H2'   | 51:ZA:1804:U:C6    | 2.55                     | 0.42              |
| 51:ZA:1839:U:H2'   | 51:ZA:1840:U:C6    | 2.55                     | 0.42              |
| 55:DB:80:THR:HG21  | 72:UB:106:ILE:HD12 | 2.02                     | 0.42              |
| 56:EB:129:ILE:HD13 | 56:EB:139:LEU:HB3  | 2.01                     | 0.42              |
| 57:FB:127:ARG:O    | 80:CC:26:GLN:NE2   | 2.53                     | 0.42              |
| 57:FB:167:LYS:HA   | 77:ZB:71:ALA:HB1   | 2.00                     | 0.42              |
| 62:KB:53:LYS:HE2   | 62:KB:53:LYS:HB3   | 1.95                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 66:OB:34:PHE:HB3   | 66:OB:41:PHE:HB2   | 2.01                     | 0.42              |
| 2:B:286:LYS:HB3    | 2:B:332:MET:HB3    | 2.02                     | 0.42              |
| 4:D:36:LEU:HG      | 4:D:50:ARG:HD2     | 2.02                     | 0.42              |
| 7:G:201:GLU:OE2    | 13:M:6:TYR:OH      | 2.30                     | 0.42              |
| 13:M:136:ASP:OD2   | 50:YA:141:C:O2'    | 2.32                     | 0.42              |
| 36:JA:37:ARG:NE    | 36:JA:38:CYS:O     | 2.53                     | 0.42              |
| 41:OA:42:CYS:HB3   | 41:OA:60:CYS:HB2   | 2.02                     | 0.42              |
| 48:WA:7:C:H2'      | 48:WA:8:U:C6       | 2.55                     | 0.42              |
| 48:WA:169:A:N1     | 48:WA:267:G:C6     | 2.88                     | 0.42              |
| 48:WA:4171:G:H4'   | 48:WA:4173:C:C2    | 2.55                     | 0.42              |
| 49:XA:3:C:H2'      | 49:XA:4:U:H6       | 1.85                     | 0.42              |
| 50:YA:30:U:H2'     | 50:YA:31:G:C8      | 2.54                     | 0.42              |
| 51:ZA:85:A:H2'     | 51:ZA:86:C:H6      | 1.85                     | 0.42              |
| 51:ZA:385:G:O2'    | 60:IB:10:LYS:NZ    | 2.51                     | 0.42              |
| 51:ZA:444:G:O6     | 60:IB:26:LYS:HE3   | 2.20                     | 0.42              |
| 51:ZA:1221:G:H2'   | 51:ZA:1222:G:H8    | 1.85                     | 0.42              |
| 51:ZA:1662:U:O4    | 51:ZA:1663:A:N6    | 2.50                     | 0.42              |
| 53:BB:65:ARG:HH12  | 66:OB:51:GLU:HG2   | 1.84                     | 0.42              |
| 57:FB:142:SER:HB2  | 80:CC:50:VAL:HG22  | 2.01                     | 0.42              |
| 60:IB:106:SER:HB3  | 60:IB:171:LEU:HG   | 2.02                     | 0.42              |
| 61:JB:149:VAL:HG11 | 61:JB:157:ILE:HD11 | 2.02                     | 0.42              |
| 73:VB:10:ASP:OD1   | 73:VB:10:ASP:N     | 2.52                     | 0.42              |
| 5:E:80:SER:OG      | 48:WA:1272:A:N1    | 2.53                     | 0.42              |
| 8:H:120:GLU:HG2    | 48:WA:4613:A:H2    | 1.85                     | 0.42              |
| 9:I:51:HIS:CD2     | 9:I:168:SER:HB2    | 2.54                     | 0.42              |
| 12:L:4:ARG:NH2     | 48:WA:4767:G:O6    | 2.33                     | 0.42              |
| 22:V:46:PRO:HB2    | 22:V:54:LEU:HD12   | 2.00                     | 0.42              |
| 29:CA:37:GLY:O     | 29:CA:41:ARG:HG3   | 2.20                     | 0.42              |
| 37:KA:8:ARG:H      | 37:KA:8:ARG:HG3    | 1.65                     | 0.42              |
| 48:WA:127:G:H2'    | 48:WA:128:C:C6     | 2.55                     | 0.42              |
| 48:WA:424:U:H2'    | 48:WA:425:U:C6     | 2.55                     | 0.42              |
| 48:WA:494:G:H2'    | 48:WA:495:C:C6     | 2.54                     | 0.42              |
| 48:WA:3722:G:H22   | 48:WA:3735:A:H2    | 1.66                     | 0.42              |
| 48:WA:3913:C:H2'   | 48:WA:3914:U:C6    | 2.54                     | 0.42              |
| 48:WA:4455:C:O2    | 48:WA:4531:G:N2    | 2.53                     | 0.42              |
| 48:WA:4752:G:H2'   | 48:WA:4753:G:H8    | 1.84                     | 0.42              |
| 51:ZA:21:U:H2'     | 51:ZA:22:A:C8      | 2.55                     | 0.42              |
| 51:ZA:28:U:H2'     | 51:ZA:29:G:H8      | 1.85                     | 0.42              |
| 51:ZA:349:A:H2'    | 51:ZA:350:C:C6     | 2.55                     | 0.42              |
| 51:ZA:991:G:C6     | 51:ZA:1134:G:H4'   | 2.55                     | 0.42              |
| 51:ZA:1620:A:OP1   | 67:PB:115:TYR:OH   | 2.35                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 67:PB:108:LYS:HG3  | 67:PB:109:PRO:HD2  | 2.01                     | 0.42              |
| 3:C:310:HIS:NE2    | 48:WA:2102:G:H2'   | 2.35                     | 0.41              |
| 14:N:25:LYS:HD2    | 14:N:25:LYS:HA     | 1.90                     | 0.41              |
| 24:X:91:ASN:OD1    | 24:X:92:GLY:N      | 2.53                     | 0.41              |
| 48:WA:469:C:H2'    | 48:WA:470:A:C8     | 2.55                     | 0.41              |
| 48:WA:2416:G:H2'   | 48:WA:2417:U:C6    | 2.54                     | 0.41              |
| 48:WA:2449:U:H2'   | 48:WA:2450:G:H8    | 1.84                     | 0.41              |
| 48:WA:2542:C:H2'   | 48:WA:2543:G:C8    | 2.55                     | 0.41              |
| 48:WA:3877:G:N1    | 48:WA:3881:G:OP1   | 2.46                     | 0.41              |
| 48:WA:4540:G:H2'   | 48:WA:4541:U:C6    | 2.55                     | 0.41              |
| 49:XA:64:G:H2'     | 49:XA:65:G:H8      | 1.84                     | 0.41              |
| 51:ZA:902:G:H2'    | 51:ZA:903:A:H8     | 1.85                     | 0.41              |
| 54:CB:128:VAL:HG11 | 54:CB:155:ILE:HG12 | 2.01                     | 0.41              |
| 54:CB:253:PRO:HA   | 54:CB:256:TRP:CD1  | 2.55                     | 0.41              |
| 58:GB:50:VAL:HG13  | 58:GB:111:LEU:HB3  | 2.01                     | 0.41              |
| 58:GB:50:VAL:HG11  | 58:GB:111:LEU:HD13 | 2.02                     | 0.41              |
| 64:MB:81:ASP:HB3   | 64:MB:84:LYS:HB2   | 2.02                     | 0.41              |
| 69:RB:37:GLU:HG3   | 84:GC:150:TRP:HE1  | 1.85                     | 0.41              |
| 70:SB:121:ARG:HG3  | 70:SB:131:VAL:HG11 | 2.01                     | 0.41              |
| 84:GC:61:GLY:HA3   | 84:GC:90:TRP:HZ2   | 1.83                     | 0.41              |
| 11:K:60:ARG:NH2    | 48:WA:72:C:N3      | 2.67                     | 0.41              |
| 26:Z:73:VAL:HB     | 26:Z:108:TYR:CG    | 2.55                     | 0.41              |
| 33:GA:17:LEU:HD12  | 33:GA:17:LEU:HA    | 1.77                     | 0.41              |
| 35:IA:52:LYS:HG2   | 35:IA:55:ARG:NH2   | 2.35                     | 0.41              |
| 48:WA:288:G:H2'    | 48:WA:289:C:C6     | 2.55                     | 0.41              |
| 48:WA:481:G:O2'    | 48:WA:483:G:OP2    | 2.33                     | 0.41              |
| 48:WA:675:G:H2'    | 48:WA:676:C:C6     | 2.55                     | 0.41              |
| 48:WA:1496:U:H2'   | 48:WA:1497:G:H8    | 1.85                     | 0.41              |
| 48:WA:1664:C:H2'   | 48:WA:1665:C:C6    | 2.55                     | 0.41              |
| 48:WA:2766:A:H2'   | 48:WA:2767:A:H8    | 1.85                     | 0.41              |
| 48:WA:3873:A:H2'   | 48:WA:3874:A:H8    | 1.86                     | 0.41              |
| 48:WA:4596:U:H2'   | 48:WA:4597:G:C8    | 2.52                     | 0.41              |
| 48:WA:5015:C:H4'   | 48:WA:5016:A:H5''  | 2.02                     | 0.41              |
| 51:ZA:799:U:H2'    | 51:ZA:800:U:C6     | 2.55                     | 0.41              |
| 51:ZA:834:C:H2'    | 51:ZA:835:C:C5     | 2.55                     | 0.41              |
| 51:ZA:921:G:OP2    | 79:BC:21:LYS:NZ    | 2.45                     | 0.41              |
| 51:ZA:1047:C:H2'   | 51:ZA:1048:G:O4'   | 2.21                     | 0.41              |
| 51:ZA:1236:G:O2'   | 67:PB:131:PRO:O    | 2.28                     | 0.41              |
| 54:CB:116:THR:OG1  | 54:CB:117:ARG:N    | 2.53                     | 0.41              |
| 55:DB:178:GLY:HA3  | 55:DB:220:LEU:HD12 | 2.03                     | 0.41              |
| 60:IB:89:GLU:O     | 60:IB:93:THR:HG22  | 2.20                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 62:KB:11:ILE:HD13  | 62:KB:11:ILE:HA    | 1.89                     | 0.41              |
| 70:SB:91:LYS:NZ    | 70:SB:109:GLU:OE1  | 2.53                     | 0.41              |
| 86:b:112:ARG:NH1   | 86:b:119:CYS:SG    | 2.93                     | 0.41              |
| 86:b:112:ARG:NE    | 86:b:121:VAL:HG11  | 2.35                     | 0.41              |
| 88:HC:338:ALA:HB2  | 88:HC:444:LYS:HD3  | 2.02                     | 0.41              |
| 9:I:158:LYS:NZ     | 48:WA:4415:C:O2    | 2.43                     | 0.41              |
| 12:L:46:ARG:HH11   | 48:WA:942:U:H5     | 1.68                     | 0.41              |
| 15:O:113:PRO:HB2   | 15:O:116:SER:HB2   | 2.02                     | 0.41              |
| 16:P:65:ARG:HH21   | 48:WA:1461:A:H5''  | 1.86                     | 0.41              |
| 17:Q:42:ARG:NH2    | 48:WA:2526:U:OP1   | 2.53                     | 0.41              |
| 17:Q:95:TRP:CE2    | 48:WA:1574:U:H4'   | 2.55                     | 0.41              |
| 18:R:87:ARG:HH11   | 49:XA:87:G:H5'     | 1.85                     | 0.41              |
| 24:X:59:ARG:NH2    | 48:WA:210:C:OP1    | 2.45                     | 0.41              |
| 25:Y:46:ILE:HG23   | 25:Y:68:ILE:HG23   | 2.02                     | 0.41              |
| 28:BA:10:SER:OG    | 28:BA:11:LEU:N     | 2.51                     | 0.41              |
| 36:JA:49:ASP:HB2   | 36:JA:52:LYS:HE2   | 2.02                     | 0.41              |
| 47:VA:26:A:O2'     | 55:DB:184:ARG:NH1  | 2.53                     | 0.41              |
| 48:WA:441:G:H2'    | 48:WA:442:G:H8     | 1.85                     | 0.41              |
| 48:WA:1174:G:H2'   | 48:WA:1175:G:C8    | 2.55                     | 0.41              |
| 48:WA:2592:G:H1'   | 48:WA:2758:G:N2    | 2.35                     | 0.41              |
| 48:WA:2618:C:H2'   | 48:WA:2619:G:H8    | 1.85                     | 0.41              |
| 48:WA:2872:A:H2'   | 48:WA:2873:A:C8    | 2.55                     | 0.41              |
| 48:WA:3772:U:H2'   | 48:WA:3773:C:C6    | 2.54                     | 0.41              |
| 51:ZA:1201:U:H2'   | 51:ZA:1202:U:C6    | 2.55                     | 0.41              |
| 51:ZA:1415:C:O2'   | 71:TB:132:ASP:OD2  | 2.25                     | 0.41              |
| 51:ZA:1862:G:O2'   | 78:AC:5:ARG:NH2    | 2.54                     | 0.41              |
| 57:FB:18:LYS:HE3   | 57:FB:46:ALA:HB3   | 2.02                     | 0.41              |
| 69:RB:99:ASP:OD1   | 69:RB:102:THR:N    | 2.41                     | 0.41              |
| 74:WB:105:THR:HG22 | 74:WB:110:ILE:HG12 | 2.03                     | 0.41              |
| 75:XB:124:LYS:HG2  | 75:XB:129:SER:HA   | 2.02                     | 0.41              |
| 88:HC:370:CYS:HA   | 88:HC:406:PRO:HA   | 2.02                     | 0.41              |
| 4:D:15:ARG:HH11    | 48:WA:1745:A:H1'   | 1.86                     | 0.41              |
| 4:D:179:ARG:HD3    | 4:D:179:ARG:HA     | 1.79                     | 0.41              |
| 19:S:4:THR:O       | 19:S:9:ARG:NE      | 2.53                     | 0.41              |
| 21:U:87:SER:HA     | 21:U:97:TYR:HB3    | 2.02                     | 0.41              |
| 41:OA:17:ARG:NH2   | 48:WA:1579:G:OP1   | 2.48                     | 0.41              |
| 48:WA:229:G:H2'    | 48:WA:230:G:C8     | 2.55                     | 0.41              |
| 48:WA:680:C:H2'    | 48:WA:681:G:C8     | 2.55                     | 0.41              |
| 48:WA:2902:U:H2'   | 48:WA:2903:G:C8    | 2.55                     | 0.41              |
| 48:WA:4995:G:C6    | 48:WA:5060:A:N1    | 2.89                     | 0.41              |
| 49:XA:3:C:H2'      | 49:XA:4:U:C6       | 2.56                     | 0.41              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 51:ZA:371:A:OP2    | 60:IB:10:LYS:HB2  | 2.20                     | 0.41              |
| 51:ZA:1415:C:H2'   | 51:ZA:1416:C:C6   | 2.55                     | 0.41              |
| 51:ZA:1713:C:H2'   | 51:ZA:1714:U:C6   | 2.55                     | 0.41              |
| 53:BB:35:ALA:HB2   | 53:BB:44:ILE:HD11 | 2.01                     | 0.41              |
| 56:EB:31:PRO:HG3   | 56:EB:43:PRO:HG3  | 2.02                     | 0.41              |
| 57:FB:192:LYS:HD3  | 57:FB:192:LYS:HA  | 1.84                     | 0.41              |
| 67:PB:52:LYS:HE3   | 67:PB:52:LYS:HB2  | 1.88                     | 0.41              |
| 88:HC:410:MET:HE2  | 88:HC:410:MET:HB3 | 1.96                     | 0.41              |
| 2:B:165:HIS:HA     | 2:B:179:HIS:O     | 2.21                     | 0.41              |
| 10:J:166:PHE:CE2   | 10:J:172:GLY:HA3  | 2.55                     | 0.41              |
| 13:M:85:VAL:HG23   | 48:WA:43:U:OP1    | 2.21                     | 0.41              |
| 26:Z:21:ARG:HB2    | 48:WA:1320:C:OP1  | 2.20                     | 0.41              |
| 42:PA:112:ARG:NH1  | 48:WA:2266:C:OP1  | 2.54                     | 0.41              |
| 43:RA:120:SER:HB3  | 86:b:48:ARG:HH21  | 1.85                     | 0.41              |
| 43:RA:146:ARG:HD3  | 43:RA:146:ARG:HA  | 1.82                     | 0.41              |
| 44:SA:8:U:O2'      | 44:SA:21:A:N1     | 2.44                     | 0.41              |
| 48:WA:126:C:H2'    | 48:WA:127:G:C8    | 2.52                     | 0.41              |
| 48:WA:1078:C:H2'   | 48:WA:1079:G:O4'  | 2.20                     | 0.41              |
| 48:WA:1347:A:H2'   | 48:WA:1348:C:C6   | 2.55                     | 0.41              |
| 48:WA:4082:C:H2'   | 48:WA:4083:G:H8   | 1.84                     | 0.41              |
| 48:WA:4265:C:H2'   | 48:WA:4266:G:O4'  | 2.21                     | 0.41              |
| 51:ZA:666:U:H2'    | 51:ZA:667:U:C6    | 2.55                     | 0.41              |
| 51:ZA:1579:A:H4'   | 51:ZA:1581:C:C5   | 2.56                     | 0.41              |
| 51:ZA:1673:U:H2'   | 51:ZA:1674:G:O4'  | 2.20                     | 0.41              |
| 56:EB:136:ILE:HG23 | 56:EB:149:TYR:CE1 | 2.56                     | 0.41              |
| 58:GB:216:ARG:HA   | 58:GB:216:ARG:HD3 | 1.91                     | 0.41              |
| 59:HB:284:THR:HG23 | 59:HB:303:PRO:HG3 | 2.02                     | 0.41              |
| 61:JB:119:LEU:HB2  | 61:JB:159:PHE:CZ  | 2.54                     | 0.41              |
| 63:LB:55:TYR:CD2   | 63:LB:115:PRO:HG2 | 2.55                     | 0.41              |
| 84:GC:90:TRP:NE1   | 84:GC:97:THR:OG1  | 2.53                     | 0.41              |
| 1:A:29:LEU:O       | 1:A:123:ARG:NH1   | 2.54                     | 0.41              |
| 3:C:60:HIS:NE2     | 3:C:100:ARG:HD3   | 2.36                     | 0.41              |
| 6:F:131:MET:O      | 6:F:135:VAL:HG22  | 2.21                     | 0.41              |
| 18:R:36:ASN:OD1    | 18:R:36:ASN:N     | 2.54                     | 0.41              |
| 42:PA:6:GLN:NE2    | 42:PA:44:ILE:O    | 2.53                     | 0.41              |
| 44:SA:41:G:O2'     | 51:ZA:1639:G:N3   | 2.53                     | 0.41              |
| 48:WA:65:A:N6      | 48:WA:75:G:H1'    | 2.36                     | 0.41              |
| 48:WA:2561:G:H2'   | 48:WA:2562:C:C6   | 2.55                     | 0.41              |
| 48:WA:2591:C:H2'   | 48:WA:2592:G:O4'  | 2.20                     | 0.41              |
| 48:WA:3600:C:H2'   | 48:WA:3601:A:H8   | 1.84                     | 0.41              |
| 48:WA:3686:G:H2'   | 48:WA:3687:C:C6   | 2.56                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 48:WA:3754:C:H2'   | 48:WA:3779:G:H5''  | 2.03                     | 0.41              |
| 48:WA:3797:A:H2'   | 48:WA:3798:U:C6    | 2.56                     | 0.41              |
| 48:WA:4091:G:H2'   | 48:WA:4092:G:C8    | 2.55                     | 0.41              |
| 51:ZA:675:U:H2'    | 51:ZA:676:C:C6     | 2.56                     | 0.41              |
| 51:ZA:953:C:H5''   | 53:BB:24:PRO:HB2   | 2.02                     | 0.41              |
| 51:ZA:1268:C:O2    | 67:PB:97:TYR:OH    | 2.38                     | 0.41              |
| 51:ZA:1446:A:H5''  | 72:UB:58:THR:HG23  | 2.02                     | 0.41              |
| 59:HB:274:LEU:HD21 | 59:HB:316:ARG:HD2  | 2.02                     | 0.41              |
| 59:HB:318:VAL:HG23 | 59:HB:330:VAL:HG13 | 2.03                     | 0.41              |
| 60:IB:114:GLU:OE2  | 60:IB:123:ARG:NH1  | 2.54                     | 0.41              |
| 84:GC:73:SER:OG    | 84:GC:117:ASN:ND2  | 2.38                     | 0.41              |
| 86:b:38:LYS:O      | 86:b:42:GLN:HG2    | 2.20                     | 0.41              |
| 6:F:126:LYS:HB2    | 19:S:133:ALA:HB3   | 2.03                     | 0.41              |
| 8:H:60:TRP:O       | 48:WA:4766:A:N6    | 2.38                     | 0.41              |
| 12:L:91:TRP:CZ2    | 48:WA:4872:G:H2'   | 2.55                     | 0.41              |
| 16:P:82:VAL:O      | 16:P:102:ALA:HA    | 2.20                     | 0.41              |
| 29:CA:26:THR:OG1   | 29:CA:85:ARG:NH1   | 2.49                     | 0.41              |
| 36:JA:41:TYR:OH    | 48:WA:2540:U:OP1   | 2.28                     | 0.41              |
| 40:NA:89:LYS:HE3   | 48:WA:4231:U:H4'   | 2.02                     | 0.41              |
| 48:WA:221:C:H2'    | 48:WA:222:C:C6     | 2.55                     | 0.41              |
| 48:WA:2664:G:H2'   | 48:WA:2665:G:H8    | 1.86                     | 0.41              |
| 48:WA:3650:A:H1'   | 48:WA:3787:A:H61   | 1.85                     | 0.41              |
| 48:WA:3915:G:H3'   | 48:WA:3916:U:H4'   | 2.02                     | 0.41              |
| 48:WA:4322:G:H2'   | 48:WA:4323:U:C6    | 2.56                     | 0.41              |
| 48:WA:4993:U:O2'   | 48:WA:4994:G:H5'   | 2.21                     | 0.41              |
| 51:ZA:21:U:O2'     | 61:JB:17:ARG:O     | 2.39                     | 0.41              |
| 51:ZA:115:U:H2'    | 51:ZA:116:U:C6     | 2.56                     | 0.41              |
| 51:ZA:304:C:OP1    | 60:IB:75:LYS:NZ    | 2.52                     | 0.41              |
| 51:ZA:388:U:H2'    | 51:ZA:389:A:H8     | 1.86                     | 0.41              |
| 51:ZA:409:C:H2'    | 51:ZA:410:G:H8     | 1.84                     | 0.41              |
| 51:ZA:832:G:N1     | 51:ZA:843:C:N3     | 2.68                     | 0.41              |
| 51:ZA:1183:A:H2'   | 51:ZA:1184:G:H8    | 1.85                     | 0.41              |
| 51:ZA:1390:U:H2'   | 51:ZA:1391:C:C6    | 2.56                     | 0.41              |
| 51:ZA:1555:U:H2'   | 51:ZA:1556:A:C8    | 2.56                     | 0.41              |
| 51:ZA:1648:G:N7    | 68:QB:43:LYS:HE2   | 2.36                     | 0.41              |
| 52:AB:124:VAL:HG21 | 52:AB:134:LEU:HD21 | 2.01                     | 0.41              |
| 52:AB:130:ASP:C    | 52:AB:133:PRO:HD2  | 2.45                     | 0.41              |
| 56:EB:212:ASP:OD1  | 56:EB:213:ALA:N    | 2.52                     | 0.41              |
| 58:GB:54:GLY:O     | 58:GB:110:ASN:ND2  | 2.54                     | 0.41              |
| 84:GC:164:ILE:HG23 | 84:GC:176:VAL:HG13 | 2.03                     | 0.41              |
| 1:A:28:ARG:HB3     | 1:A:123:ARG:HB3    | 2.03                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:B:389:MET:O     | 48:WA:5043:G:N1    | 2.51                     | 0.41              |
| 5:E:287:HIS:CE1   | 31:EA:33:VAL:HG22  | 2.56                     | 0.41              |
| 7:G:119:GLN:HG3   | 13:M:28:TRP:CH2    | 2.55                     | 0.41              |
| 13:M:108:ARG:HB2  | 13:M:161:MET:HE1   | 2.03                     | 0.41              |
| 24:X:51:LYS:HB2   | 50:YA:72:A:OP2     | 2.21                     | 0.41              |
| 25:Y:30:ASP:OD1   | 25:Y:30:ASP:N      | 2.51                     | 0.41              |
| 33:GA:84:ARG:NH2  | 48:WA:17:A:OP1     | 2.37                     | 0.41              |
| 48:WA:269:G:H2'   | 48:WA:270:U:C6     | 2.56                     | 0.41              |
| 48:WA:440:U:H2'   | 48:WA:441:G:H8     | 1.85                     | 0.41              |
| 48:WA:1648:A:H2'  | 48:WA:1649:U:C6    | 2.56                     | 0.41              |
| 48:WA:1872:C:H2'  | 48:WA:1873:A:C8    | 2.56                     | 0.41              |
| 48:WA:2266:C:H2'  | 48:WA:2267:G:O4'   | 2.20                     | 0.41              |
| 48:WA:2599:G:H2'  | 48:WA:2600:A:H8    | 1.85                     | 0.41              |
| 48:WA:3650:A:H1'  | 48:WA:3787:A:N6    | 2.36                     | 0.41              |
| 48:WA:3776:A:H2'  | 48:WA:3777:A:C8    | 2.54                     | 0.41              |
| 51:ZA:158:A:H2'   | 51:ZA:159:A:O4'    | 2.20                     | 0.41              |
| 51:ZA:429:C:H2'   | 51:ZA:430:C:C6     | 2.56                     | 0.41              |
| 51:ZA:1683:C:N3   | 80:CC:24:GLN:HG3   | 2.36                     | 0.41              |
| 51:ZA:1688:C:H2'  | 51:ZA:1689:C:C6    | 2.56                     | 0.41              |
| 55:DB:144:ARG:HG3 | 55:DB:213:VAL:HG13 | 2.03                     | 0.41              |
| 56:EB:221:ARG:O   | 56:EB:225:ILE:HG12 | 2.20                     | 0.41              |
| 57:FB:35:LEU:HD23 | 57:FB:39:ILE:HD11  | 2.03                     | 0.41              |
| 88:HC:342:ALA:HB3 | 88:HC:404:MET:HE1  | 2.03                     | 0.41              |
| 7:G:159:THR:HG22  | 7:G:248:HIS:NE2    | 2.35                     | 0.41              |
| 10:J:96:LYS:O     | 10:J:159:LYS:NZ    | 2.41                     | 0.41              |
| 11:K:62:PRO:HG3   | 48:WA:74:G:H1'     | 2.03                     | 0.41              |
| 11:K:124:LEU:HD11 | 33:GA:119:TYR:HB2  | 2.01                     | 0.41              |
| 14:N:14:HIS:CE1   | 14:N:119:VAL:HG13  | 2.56                     | 0.41              |
| 15:O:91:ARG:NH1   | 48:WA:423:G:OP1    | 2.48                     | 0.41              |
| 17:Q:18:GLY:HA3   | 48:WA:2824:G:H5''  | 2.02                     | 0.41              |
| 18:R:21:LYS:HE2   | 18:R:21:LYS:HB2    | 1.87                     | 0.41              |
| 18:R:107:THR:O    | 18:R:111:ARG:HG2   | 2.20                     | 0.41              |
| 26:Z:12:ARG:NH1   | 48:WA:2347:G:OP2   | 2.54                     | 0.41              |
| 26:Z:24:LYS:HD3   | 26:Z:26:ARG:HH21   | 1.86                     | 0.41              |
| 43:RA:104:ILE:HB  | 43:RA:143:VAL:HG22 | 2.03                     | 0.41              |
| 43:RA:146:ARG:O   | 43:RA:149:HIS:ND1  | 2.38                     | 0.41              |
| 44:SA:11:U:H2'    | 44:SA:12:G:C8      | 2.55                     | 0.41              |
| 46:UA:28:U:H2'    | 46:UA:29:C:C6      | 2.55                     | 0.41              |
| 48:WA:221:C:H2'   | 48:WA:222:C:H6     | 1.85                     | 0.41              |
| 48:WA:368:C:H2'   | 48:WA:369:G:C8     | 2.56                     | 0.41              |
| 48:WA:475:G:H2'   | 48:WA:476:G:C8     | 2.56                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 48:WA:1444:C:H2'   | 48:WA:1445:A:C8    | 2.56                     | 0.41              |
| 48:WA:1481:G:H2'   | 48:WA:1482:C:C6    | 2.55                     | 0.41              |
| 48:WA:1506:G:H2'   | 48:WA:1507:C:H6    | 1.85                     | 0.41              |
| 48:WA:2287:A:H2'   | 48:WA:2288:G:C8    | 2.55                     | 0.41              |
| 48:WA:4455:C:H1'   | 48:WA:4531:G:H22   | 1.85                     | 0.41              |
| 51:ZA:65:C:P       | 58:GB:175:LYS:H    | 2.43                     | 0.41              |
| 51:ZA:162:C:H2'    | 51:ZA:163:U:O4'    | 2.21                     | 0.41              |
| 51:ZA:220:U:H2'    | 51:ZA:221:A:C8     | 2.56                     | 0.41              |
| 51:ZA:495:U:H2'    | 51:ZA:496:C:O4'    | 2.21                     | 0.41              |
| 51:ZA:877:C:H2'    | 51:ZA:878:G:C8     | 2.56                     | 0.41              |
| 51:ZA:916:A:C6     | 65:NB:73:ARG:HD3   | 2.56                     | 0.41              |
| 51:ZA:944:A:H2'    | 51:ZA:945:U:H6     | 1.86                     | 0.41              |
| 51:ZA:1005:G:OP2   | 53:BB:162:ARG:NH1  | 2.54                     | 0.41              |
| 51:ZA:1284:A:C5    | 64:MB:91:LEU:HD11  | 2.56                     | 0.41              |
| 51:ZA:1403:C:H42   | 51:ZA:1432:U:P     | 2.43                     | 0.41              |
| 52:AB:102:ARG:HA   | 52:AB:102:ARG:HD2  | 1.83                     | 0.41              |
| 53:BB:180:ASP:OD1  | 53:BB:180:ASP:N    | 2.52                     | 0.41              |
| 55:DB:134:LEU:HD12 | 55:DB:236:ILE:HG12 | 2.02                     | 0.41              |
| 57:FB:55:ARG:HG2   | 68:QB:151:ARG:HD3  | 2.01                     | 0.41              |
| 58:GB:121:ILE:HG22 | 58:GB:123:GLY:H    | 1.86                     | 0.41              |
| 59:HB:248:LYS:HD2  | 59:HB:248:LYS:HA   | 1.92                     | 0.41              |
| 65:NB:83:ASP:OD1   | 65:NB:83:ASP:N     | 2.54                     | 0.41              |
| 65:NB:87:ASP:OD1   | 65:NB:87:ASP:N     | 2.54                     | 0.41              |
| 66:OB:127:GLY:HA2  | 78:AC:58:VAL:HG22  | 2.02                     | 0.41              |
| 75:XB:52:LEU:HD11  | 75:XB:71:ARG:HD3   | 2.03                     | 0.41              |
| 80:CC:20:ARG:NH2   | 80:CC:25:GLY:O     | 2.54                     | 0.41              |
| 84:GC:130:LYS:HG2  | 84:GC:141:THR:HB   | 2.02                     | 0.41              |
| 86:b:125:ALA:HA    | 86:b:218:GLY:HA2   | 2.02                     | 0.41              |
| 1:A:181:LYS:HB2    | 48:WA:1579:G:C5    | 2.56                     | 0.41              |
| 3:C:149:GLU:HG2    | 3:C:151:PRO:HD2    | 2.03                     | 0.41              |
| 4:D:215:ASP:OD1    | 4:D:215:ASP:N      | 2.54                     | 0.41              |
| 6:F:70:MET:HA      | 6:F:73:MET:HG2     | 2.03                     | 0.41              |
| 8:H:91:LYS:HB2     | 8:H:183:GLU:HB3    | 2.03                     | 0.41              |
| 9:I:177:ASN:HB2    | 9:I:180:GLU:HG3    | 2.01                     | 0.41              |
| 19:S:54:HIS:ND1    | 19:S:56:CYS:SG     | 2.82                     | 0.41              |
| 21:U:48:ARG:HB3    | 21:U:51:ARG:HE     | 1.86                     | 0.41              |
| 40:NA:9:ARG:HA     | 40:NA:20:PRO:HA    | 2.02                     | 0.41              |
| 43:RA:97:ASN:ND2   | 48:WA:1981:A:OP1   | 2.54                     | 0.41              |
| 44:SA:50:U:H2'     | 44:SA:51:C:C6      | 2.56                     | 0.41              |
| 48:WA:440:U:H2'    | 48:WA:441:G:C8     | 2.56                     | 0.41              |
| 48:WA:1255:G:H1    | 48:WA:1262:G:N2    | 2.18                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 48:WA:1310:C:H2'  | 48:WA:1311:C:C6    | 2.56                     | 0.41              |
| 48:WA:1346:C:H2'  | 48:WA:1347:A:H8    | 1.86                     | 0.41              |
| 48:WA:2540:U:H2'  | 48:WA:2541:C:C6    | 2.56                     | 0.41              |
| 48:WA:4091:G:H2'  | 48:WA:4092:G:H8    | 1.86                     | 0.41              |
| 51:ZA:26:U:H2'    | 51:ZA:27:A:C8      | 2.55                     | 0.41              |
| 51:ZA:1617:G:N7   | 67:PB:47:ARG:NH1   | 2.69                     | 0.41              |
| 84:GC:152:SER:H   | 84:GC:169:GLY:HA2  | 1.85                     | 0.41              |
| 88:HC:341:THR:HB  | 88:HC:440:ALA:HB3  | 2.03                     | 0.41              |
| 13:M:63:ARG:NH1   | 13:M:131:GLU:OE2   | 2.54                     | 0.40              |
| 16:P:18:PRO:HG3   | 16:P:29:VAL:HG21   | 2.04                     | 0.40              |
| 16:P:178:ARG:H    | 26:Z:51:GLY:HA2    | 1.84                     | 0.40              |
| 29:CA:23:ARG:HG2  | 29:CA:121:ASN:HA   | 2.03                     | 0.40              |
| 48:WA:913:U:H2'   | 48:WA:914:G:O4'    | 2.21                     | 0.40              |
| 48:WA:1293:G:H2'  | 48:WA:1294:C:C6    | 2.56                     | 0.40              |
| 48:WA:1336:A:H2'  | 48:WA:1337:G:H8    | 1.86                     | 0.40              |
| 48:WA:2786:C:H2'  | 48:WA:2787:C:C6    | 2.57                     | 0.40              |
| 48:WA:3929:U:H2'  | 48:WA:3930:A:C8    | 2.56                     | 0.40              |
| 48:WA:5007:G:H22  | 48:WA:5043:G:H1'   | 1.86                     | 0.40              |
| 51:ZA:199:C:O2'   | 51:ZA:200:G:H5'    | 2.21                     | 0.40              |
| 51:ZA:561:A:H5''  | 61:JB:173:VAL:HG12 | 2.03                     | 0.40              |
| 51:ZA:1143:A:O3'  | 51:ZA:1355:C:N4    | 2.54                     | 0.40              |
| 51:ZA:1338:G:H2'  | 51:ZA:1339:U:C6    | 2.56                     | 0.40              |
| 58:GB:160:LYS:HD2 | 58:GB:161:PRO:HD2  | 2.03                     | 0.40              |
| 86:b:13:TYR:HA    | 86:b:16:LYS:HE2    | 2.03                     | 0.40              |
| 88:HC:335:MET:HE3 | 88:HC:443:LYS:HD2  | 2.03                     | 0.40              |
| 1:A:210:PRO:HG2   | 1:A:235:VAL:HG11   | 2.03                     | 0.40              |
| 6:F:221:LYS:HB3   | 6:F:230:GLY:HA2    | 2.03                     | 0.40              |
| 22:V:110:ARG:HA   | 22:V:113:LYS:HG2   | 2.03                     | 0.40              |
| 30:DA:44:ARG:NH2  | 48:WA:1314:A:O2'   | 2.55                     | 0.40              |
| 35:IA:2:THR:O     | 35:IA:7:SER:OG     | 2.29                     | 0.40              |
| 45:TA:43:A:H2'    | 45:TA:44:G:C8      | 2.56                     | 0.40              |
| 48:WA:926:C:H2'   | 48:WA:927:C:C6     | 2.56                     | 0.40              |
| 48:WA:1658:U:H2'  | 48:WA:1659:G:H8    | 1.86                     | 0.40              |
| 48:WA:2731:C:H2'  | 48:WA:2732:U:C6    | 2.56                     | 0.40              |
| 48:WA:3709:U:H2'  | 48:WA:3710:C:H6    | 1.86                     | 0.40              |
| 49:XA:15:C:H2'    | 49:XA:16:A:C8      | 2.56                     | 0.40              |
| 49:XA:58:A:H2'    | 49:XA:59:G:H8      | 1.86                     | 0.40              |
| 51:ZA:569:A:H2'   | 51:ZA:570:C:H6     | 1.86                     | 0.40              |
| 51:ZA:1139:C:N4   | 51:ZA:1149:A:H62   | 2.20                     | 0.40              |
| 51:ZA:1198:G:H2'  | 51:ZA:1199:A:H8    | 1.85                     | 0.40              |
| 51:ZA:1579:A:H4'  | 51:ZA:1581:C:H5    | 1.86                     | 0.40              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 54:CB:142:LYS:HG2 | 54:CB:153:GLY:HA3  | 2.02                     | 0.40              |
| 54:CB:166:ARG:HB2 | 54:CB:248:TYR:CG   | 2.56                     | 0.40              |
| 55:DB:93:THR:HA   | 55:DB:96:VAL:HG12  | 2.03                     | 0.40              |
| 61:JB:133:ARG:HB3 | 61:JB:143:ASN:HD22 | 1.86                     | 0.40              |
| 69:RB:76:GLU:HA   | 69:RB:79:GLU:HG3   | 2.03                     | 0.40              |
| 71:TB:42:HIS:NE2  | 71:TB:43:LYS:HE3   | 2.36                     | 0.40              |
| 74:WB:3:ARG:HD3   | 74:WB:6:VAL:HG12   | 2.02                     | 0.40              |
| 78:AC:38:LYS:HG2  | 78:AC:40:VAL:HG23  | 2.04                     | 0.40              |
| 84:GC:78:ALA:HB2  | 84:GC:92:LEU:HD11  | 2.03                     | 0.40              |
| 3:C:230:LEU:HD21  | 3:C:239:LYS:HD2    | 2.03                     | 0.40              |
| 6:F:88:LEU:HD11   | 6:F:121:PHE:HB3    | 2.03                     | 0.40              |
| 16:P:85:THR:HG22  | 16:P:104:ARG:HB2   | 2.03                     | 0.40              |
| 16:P:91:ARG:HB3   | 26:Z:76:ASP:HB3    | 2.03                     | 0.40              |
| 28:BA:22:MET:HE1  | 28:BA:29:LEU:HD21  | 2.03                     | 0.40              |
| 30:DA:37:LYS:HD2  | 30:DA:38:PRO:HD2   | 2.03                     | 0.40              |
| 46:UA:27:U:H2'    | 46:UA:28:U:C6      | 2.57                     | 0.40              |
| 48:WA:263:G:H2'   | 48:WA:264:C:C6     | 2.57                     | 0.40              |
| 48:WA:312:G:H1    | 48:WA:325:U:H3     | 1.69                     | 0.40              |
| 48:WA:1363:G:H2'  | 48:WA:1364:G:H8    | 1.85                     | 0.40              |
| 48:WA:1741:G:H2'  | 48:WA:1742:C:C6    | 2.56                     | 0.40              |
| 48:WA:4870:G:O2'  | 48:WA:4874:G:OP1   | 2.37                     | 0.40              |
| 51:ZA:1623:A:C6   | 70:SB:132:ARG:HD3  | 2.56                     | 0.40              |
| 51:ZA:1627:C:H2'  | 51:ZA:1628:C:H6    | 1.86                     | 0.40              |
| 60:IB:157:LYS:NZ  | 60:IB:158:ILE:O    | 2.51                     | 0.40              |
| 62:KB:64:TRP:CD2  | 81:DC:23:VAL:HG22  | 2.56                     | 0.40              |
| 64:MB:19:GLN:OE1  | 64:MB:88:TRP:HB3   | 2.21                     | 0.40              |
| 84:GC:35:SER:OG   | 84:GC:36:ARG:N     | 2.54                     | 0.40              |
| 7:G:158:GLU:HB2   | 7:G:162:GLU:HB2    | 2.02                     | 0.40              |
| 13:M:46:ASP:OD1   | 13:M:46:ASP:N      | 2.54                     | 0.40              |
| 13:M:123:GLU:OE1  | 13:M:128:LYS:NZ    | 2.54                     | 0.40              |
| 14:N:121:PRO:HD3  | 18:R:168:THR:HG22  | 2.03                     | 0.40              |
| 16:P:11:ARG:HG3   | 48:WA:2083:C:H5''  | 2.03                     | 0.40              |
| 23:W:56:ARG:HE    | 48:WA:14:C:P       | 2.44                     | 0.40              |
| 24:X:106:ILE:HG21 | 24:X:109:LEU:HD23  | 2.03                     | 0.40              |
| 26:Z:113:GLY:N    | 26:Z:133:ALA:HB2   | 2.36                     | 0.40              |
| 31:EA:100:ARG:HG2 | 48:WA:4755:U:OP2   | 2.22                     | 0.40              |
| 33:GA:109:ARG:NH2 | 48:WA:267:G:OP1    | 2.45                     | 0.40              |
| 43:RA:128:THR:O   | 43:RA:131:GLU:HG2  | 2.22                     | 0.40              |
| 48:WA:751:G:O2'   | 48:WA:914:G:N1     | 2.51                     | 0.40              |
| 48:WA:753:G:H3'   | 48:WA:754:G:H8     | 1.86                     | 0.40              |
| 48:WA:1859:C:H2'  | 48:WA:1860:A:C8    | 2.57                     | 0.40              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 48:WA:2685:C:H2'  | 48:WA:2686:C:C6    | 2.57                     | 0.40              |
| 48:WA:2762:G:H4'  | 48:WA:2763:U:H5'   | 2.03                     | 0.40              |
| 48:WA:2782:C:H2'  | 48:WA:2783:G:H8    | 1.85                     | 0.40              |
| 48:WA:3600:C:H2'  | 48:WA:3601:A:C8    | 2.56                     | 0.40              |
| 48:WA:4175:G:H2'  | 48:WA:4176:U:C6    | 2.56                     | 0.40              |
| 48:WA:4942:C:H5'  | 48:WA:4943:G:H5''  | 2.03                     | 0.40              |
| 50:YA:26:C:H2'    | 50:YA:27:U:C6      | 2.57                     | 0.40              |
| 51:ZA:316:G:H2'   | 51:ZA:317:C:C6     | 2.56                     | 0.40              |
| 51:ZA:568:C:H42   | 51:ZA:582:U:H3     | 1.69                     | 0.40              |
| 51:ZA:1033:G:N1   | 51:ZA:1080:A:O2'   | 2.43                     | 0.40              |
| 51:ZA:1221:G:H2'  | 51:ZA:1222:G:C8    | 2.56                     | 0.40              |
| 51:ZA:1380:C:H2'  | 51:ZA:1381:G:C8    | 2.56                     | 0.40              |
| 52:AB:137:ALA:HA  | 52:AB:142:LEU:HB3  | 2.02                     | 0.40              |
| 56:EB:59:ASP:O    | 56:EB:63:LYS:HG2   | 2.22                     | 0.40              |
| 56:EB:155:LYS:HA  | 56:EB:155:LYS:HD3  | 1.88                     | 0.40              |
| 65:NB:40:LEU:HD12 | 65:NB:50:ILE:HG23  | 2.04                     | 0.40              |
| 74:WB:93:LEU:HB2  | 74:WB:102:ILE:HD11 | 2.04                     | 0.40              |
| 75:XB:142:ARG:HA  | 75:XB:142:ARG:HH11 | 1.86                     | 0.40              |
| 78:AC:37:LYS:HB2  | 78:AC:37:LYS:HE3   | 1.84                     | 0.40              |
| 78:AC:45:VAL:HG11 | 78:AC:53:ILE:HG13  | 2.03                     | 0.40              |
| 84:GC:261:LEU:O   | 84:GC:264:LYS:NZ   | 2.38                     | 0.40              |
| 87:c:242:GLU:O    | 87:c:246:GLU:HB2   | 2.21                     | 0.40              |
| 2:B:373:LYS:HD2   | 48:WA:4629:U:H4'   | 2.04                     | 0.40              |
| 3:C:65:GLU:HB3    | 3:C:80:ARG:HD3     | 2.03                     | 0.40              |
| 3:C:286:ASN:N     | 16:P:124:ASP:OD2   | 2.55                     | 0.40              |
| 5:E:193:HIS:HB3   | 5:E:196:PHE:HD2    | 1.87                     | 0.40              |
| 6:F:175:ALA:HB1   | 48:WA:2104:G:C8    | 2.57                     | 0.40              |
| 9:I:193:ASP:OD2   | 48:WA:1752:G:N2    | 2.53                     | 0.40              |
| 18:R:35:PRO:HD2   | 18:R:39:VAL:HG21   | 2.03                     | 0.40              |
| 21:U:89:ARG:HB2   | 21:U:95:PHE:CE2    | 2.56                     | 0.40              |
| 33:GA:89:ARG:CZ   | 33:GA:93:ARG:HH12  | 2.34                     | 0.40              |
| 48:WA:227:A:N6    | 48:WA:242:U:O4'    | 2.54                     | 0.40              |
| 48:WA:273:U:H2'   | 48:WA:274:C:C6     | 2.56                     | 0.40              |
| 48:WA:441:G:H2'   | 48:WA:442:G:C8     | 2.57                     | 0.40              |
| 48:WA:456:C:H2'   | 48:WA:457:G:H8     | 1.84                     | 0.40              |
| 48:WA:457:G:H2'   | 48:WA:458:C:C6     | 2.55                     | 0.40              |
| 48:WA:1380:C:H4'  | 48:WA:1381:C:H5'   | 2.04                     | 0.40              |
| 48:WA:1867:G:N2   | 48:WA:1870:A:OP2   | 2.43                     | 0.40              |
| 48:WA:2001:A:N6   | 86:b:44:ARG:HH21   | 2.20                     | 0.40              |
| 48:WA:2294:C:H2'  | 48:WA:2295:U:C6    | 2.57                     | 0.40              |
| 48:WA:2635:U:H2'  | 48:WA:2636:C:C6    | 2.57                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 48:WA:4553:U:H2'  | 48:WA:4554:U:C6   | 2.56                     | 0.40              |
| 51:ZA:49:C:H2'    | 51:ZA:472:C:H41   | 1.86                     | 0.40              |
| 51:ZA:651:U:H2'   | 51:ZA:652:U:C6    | 2.57                     | 0.40              |
| 51:ZA:842:C:H2'   | 51:ZA:843:C:C6    | 2.56                     | 0.40              |
| 51:ZA:1089:G:O6   | 75:XB:3:LYS:NZ    | 2.37                     | 0.40              |
| 51:ZA:1202:U:H2'  | 51:ZA:1203:G:C8   | 2.56                     | 0.40              |
| 71:TB:38:LYS:NZ   | 71:TB:40:ALA:O    | 2.43                     | 0.40              |
| 76:YB:29:HIS:O    | 76:YB:29:HIS:ND1  | 2.55                     | 0.40              |
| 84:GC:31:ILE:HD12 | 84:GC:299:PHE:CD2 | 2.57                     | 0.40              |
| 86:b:54:LEU:HD22  | 86:b:54:LEU:HA    | 1.91                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1   | A     | 248/257 (96%) | 236 (95%) | 12 (5%) | 0        | 100         | 100 |
| 2   | B     | 395/403 (98%) | 383 (97%) | 12 (3%) | 0        | 100         | 100 |
| 3   | C     | 360/413 (87%) | 348 (97%) | 12 (3%) | 0        | 100         | 100 |
| 4   | D     | 292/297 (98%) | 286 (98%) | 6 (2%)  | 0        | 100         | 100 |
| 5   | E     | 222/291 (76%) | 217 (98%) | 5 (2%)  | 0        | 100         | 100 |
| 6   | F     | 225/249 (90%) | 219 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 7   | G     | 225/319 (70%) | 220 (98%) | 5 (2%)  | 0        | 100         | 100 |
| 8   | H     | 188/192 (98%) | 182 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 9   | I     | 201/214 (94%) | 196 (98%) | 5 (2%)  | 0        | 100         | 100 |
| 10  | J     | 169/178 (95%) | 167 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 11  | K     | 208/211 (99%) | 202 (97%) | 6 (3%)  | 0        | 100         | 100 |
| 12  | L     | 136/218 (62%) | 132 (97%) | 4 (3%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 13  | M     | 201/204 (98%) | 198 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 14  | N     | 197/203 (97%) | 195 (99%) | 2 (1%)  | 0        | 100         | 100 |
| 15  | O     | 154/213 (72%) | 151 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 16  | P     | 185/188 (98%) | 181 (98%) | 4 (2%)  | 0        | 100         | 100 |
| 17  | Q     | 178/212 (84%) | 174 (98%) | 4 (2%)  | 0        | 100         | 100 |
| 18  | R     | 174/224 (78%) | 166 (95%) | 8 (5%)  | 0        | 100         | 100 |
| 19  | S     | 157/160 (98%) | 152 (97%) | 5 (3%)  | 0        | 100         | 100 |
| 20  | T     | 99/128 (77%)  | 96 (97%)  | 3 (3%)  | 0        | 100         | 100 |
| 21  | U     | 133/140 (95%) | 129 (97%) | 4 (3%)  | 0        | 100         | 100 |
| 22  | V     | 106/157 (68%) | 104 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 23  | W     | 116/156 (74%) | 115 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 24  | X     | 132/145 (91%) | 128 (97%) | 4 (3%)  | 0        | 100         | 100 |
| 25  | Y     | 133/136 (98%) | 131 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 26  | Z     | 145/148 (98%) | 141 (97%) | 4 (3%)  | 0        | 100         | 100 |
| 27  | AA    | 103/245 (42%) | 101 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 28  | BA    | 97/115 (84%)  | 95 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 29  | CA    | 106/125 (85%) | 104 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 30  | DA    | 127/135 (94%) | 124 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 31  | EA    | 107/110 (97%) | 106 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 32  | FA    | 112/129 (87%) | 111 (99%) | 1 (1%)  | 0        | 100         | 100 |
| 33  | GA    | 119/123 (97%) | 117 (98%) | 2 (2%)  | 0        | 100         | 100 |
| 34  | HA    | 100/105 (95%) | 93 (93%)  | 7 (7%)  | 0        | 100         | 100 |
| 35  | IA    | 85/97 (88%)   | 84 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 36  | JA    | 67/70 (96%)   | 65 (97%)  | 2 (3%)  | 0        | 100         | 100 |
| 37  | KA    | 48/51 (94%)   | 46 (96%)  | 2 (4%)  | 0        | 100         | 100 |
| 38  | LA    | 50/128 (39%)  | 49 (98%)  | 1 (2%)  | 0        | 100         | 100 |
| 39  | MA    | 23/25 (92%)   | 23 (100%) | 0       | 0        | 100         | 100 |
| 40  | NA    | 102/106 (96%) | 98 (96%)  | 4 (4%)  | 0        | 100         | 100 |
| 41  | OA    | 89/92 (97%)   | 86 (97%)  | 3 (3%)  | 0        | 100         | 100 |
| 42  | PA    | 122/137 (89%) | 119 (98%) | 3 (2%)  | 0        | 100         | 100 |
| 43  | RA    | 151/165 (92%) | 140 (93%) | 11 (7%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|------------|---------|----------|-------------|-----|
| 52  | AB    | 215/295 (73%) | 213 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 53  | BB    | 211/264 (80%) | 207 (98%)  | 4 (2%)  | 0        | 100         | 100 |
| 54  | CB    | 218/293 (74%) | 213 (98%)  | 5 (2%)  | 0        | 100         | 100 |
| 55  | DB    | 226/281 (80%) | 225 (100%) | 1 (0%)  | 0        | 100         | 100 |
| 56  | EB    | 260/263 (99%) | 251 (96%)  | 9 (4%)  | 0        | 100         | 100 |
| 57  | FB    | 181/204 (89%) | 175 (97%)  | 6 (3%)  | 0        | 100         | 100 |
| 58  | GB    | 235/249 (94%) | 231 (98%)  | 4 (2%)  | 0        | 100         | 100 |
| 59  | HB    | 181/432 (42%) | 176 (97%)  | 5 (3%)  | 0        | 100         | 100 |
| 60  | IB    | 204/208 (98%) | 201 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 61  | JB    | 183/194 (94%) | 179 (98%)  | 4 (2%)  | 0        | 100         | 100 |
| 62  | KB    | 94/165 (57%)  | 92 (98%)   | 2 (2%)  | 0        | 100         | 100 |
| 63  | LB    | 140/158 (89%) | 136 (97%)  | 4 (3%)  | 0        | 100         | 100 |
| 64  | MB    | 115/132 (87%) | 109 (95%)  | 6 (5%)  | 0        | 100         | 100 |
| 65  | NB    | 147/151 (97%) | 146 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 66  | OB    | 134/151 (89%) | 130 (97%)  | 4 (3%)  | 0        | 100         | 100 |
| 67  | PB    | 127/145 (88%) | 125 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 68  | QB    | 140/172 (81%) | 136 (97%)  | 4 (3%)  | 0        | 100         | 100 |
| 69  | RB    | 130/135 (96%) | 127 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 70  | SB    | 142/152 (93%) | 139 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 71  | TB    | 140/145 (97%) | 135 (96%)  | 5 (4%)  | 0        | 100         | 100 |
| 72  | UB    | 100/119 (84%) | 97 (97%)   | 3 (3%)  | 0        | 100         | 100 |
| 73  | VB    | 81/83 (98%)   | 78 (96%)   | 3 (4%)  | 0        | 100         | 100 |
| 74  | WB    | 127/130 (98%) | 123 (97%)  | 4 (3%)  | 0        | 100         | 100 |
| 75  | XB    | 139/143 (97%) | 135 (97%)  | 4 (3%)  | 0        | 100         | 100 |
| 76  | YB    | 122/131 (93%) | 120 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 77  | ZB    | 83/124 (67%)  | 82 (99%)   | 1 (1%)  | 0        | 100         | 100 |
| 78  | AC    | 99/115 (86%)  | 96 (97%)   | 3 (3%)  | 0        | 100         | 100 |
| 79  | BC    | 81/84 (96%)   | 79 (98%)   | 2 (2%)  | 0        | 100         | 100 |
| 80  | CC    | 60/69 (87%)   | 60 (100%)  | 0       | 0        | 100         | 100 |
| 81  | DC    | 53/56 (95%)   | 53 (100%)  | 0       | 0        | 100         | 100 |
| 82  | EC    | 53/133 (40%)  | 51 (96%)   | 2 (4%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Favoured    | Allowed  | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 83  | FC    | 67/188 (36%)      | 63 (94%)    | 4 (6%)   | 0        | 100         | 100 |
| 84  | GC    | 311/317 (98%)     | 301 (97%)   | 10 (3%)  | 0        | 100         | 100 |
| 85  | IC    | 2/4 (50%)         | 2 (100%)    | 0        | 0        | 100         | 100 |
| 86  | b     | 162/318 (51%)     | 152 (94%)   | 9 (6%)   | 1 (1%)   | 21          | 52  |
| 87  | c     | 12/14 (86%)       | 12 (100%)   | 0        | 0        | 100         | 100 |
| 88  | HC    | 221/462 (48%)     | 209 (95%)   | 12 (5%)  | 0        | 100         | 100 |
| All | All   | 11783/14293 (82%) | 11469 (97%) | 313 (3%) | 1 (0%)   | 100         | 100 |

All (1) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 86  | b     | 225 | VAL  |

### 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   | A     | 192/199 (96%) | 191 (100%) | 1 (0%)   | 81          | 85  |
| 2   | B     | 344/348 (99%) | 337 (98%)  | 7 (2%)   | 48          | 72  |
| 3   | C     | 302/337 (90%) | 300 (99%)  | 2 (1%)   | 76          | 82  |
| 4   | D     | 247/250 (99%) | 246 (100%) | 1 (0%)   | 84          | 86  |
| 5   | E     | 201/251 (80%) | 199 (99%)  | 2 (1%)   | 68          | 79  |
| 6   | F     | 198/218 (91%) | 198 (100%) | 0        | 100         | 100 |
| 7   | G     | 197/273 (72%) | 194 (98%)  | 3 (2%)   | 57          | 75  |
| 8   | H     | 169/171 (99%) | 165 (98%)  | 4 (2%)   | 43          | 69  |
| 9   | I     | 175/181 (97%) | 173 (99%)  | 2 (1%)   | 65          | 78  |
| 10  | J     | 144/149 (97%) | 142 (99%)  | 2 (1%)   | 59          | 76  |
| 11  | K     | 175/176 (99%) | 171 (98%)  | 4 (2%)   | 44          | 70  |
| 12  | L     | 117/161 (73%) | 117 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Rotameric  | Outliers | Percentiles |     |
|-----|-------|---------------|------------|----------|-------------|-----|
| 13  | M     | 171/172 (99%) | 167 (98%)  | 4 (2%)   | 44          | 70  |
| 14  | N     | 171/173 (99%) | 171 (100%) | 0        | 100         | 100 |
| 15  | O     | 137/190 (72%) | 137 (100%) | 0        | 100         | 100 |
| 16  | P     | 164/165 (99%) | 162 (99%)  | 2 (1%)   | 63          | 78  |
| 17  | Q     | 159/191 (83%) | 159 (100%) | 0        | 100         | 100 |
| 18  | R     | 157/192 (82%) | 153 (98%)  | 4 (2%)   | 42          | 69  |
| 19  | S     | 139/140 (99%) | 137 (99%)  | 2 (1%)   | 59          | 76  |
| 20  | T     | 91/114 (80%)  | 91 (100%)  | 0        | 100         | 100 |
| 21  | U     | 103/107 (96%) | 101 (98%)  | 2 (2%)   | 50          | 73  |
| 22  | V     | 89/126 (71%)  | 88 (99%)   | 1 (1%)   | 65          | 78  |
| 23  | W     | 106/134 (79%) | 105 (99%)  | 1 (1%)   | 70          | 80  |
| 24  | X     | 124/135 (92%) | 120 (97%)  | 4 (3%)   | 34          | 64  |
| 25  | Y     | 117/118 (99%) | 116 (99%)  | 1 (1%)   | 70          | 80  |
| 26  | Z     | 119/120 (99%) | 118 (99%)  | 1 (1%)   | 73          | 81  |
| 27  | AA    | 87/184 (47%)  | 87 (100%)  | 0        | 100         | 100 |
| 28  | BA    | 85/98 (87%)   | 83 (98%)   | 2 (2%)   | 43          | 69  |
| 29  | CA    | 98/110 (89%)  | 98 (100%)  | 0        | 100         | 100 |
| 30  | DA    | 115/121 (95%) | 114 (99%)  | 1 (1%)   | 70          | 80  |
| 31  | EA    | 88/89 (99%)   | 88 (100%)  | 0        | 100         | 100 |
| 32  | FA    | 98/109 (90%)  | 95 (97%)   | 3 (3%)   | 35          | 64  |
| 33  | GA    | 109/110 (99%) | 106 (97%)  | 3 (3%)   | 38          | 66  |
| 34  | HA    | 86/89 (97%)   | 86 (100%)  | 0        | 100         | 100 |
| 35  | IA    | 74/80 (92%)   | 73 (99%)   | 1 (1%)   | 59          | 76  |
| 36  | JA    | 64/65 (98%)   | 64 (100%)  | 0        | 100         | 100 |
| 37  | KA    | 47/48 (98%)   | 46 (98%)   | 1 (2%)   | 47          | 71  |
| 38  | LA    | 48/116 (41%)  | 47 (98%)   | 1 (2%)   | 47          | 71  |
| 39  | MA    | 24/24 (100%)  | 24 (100%)  | 0        | 100         | 100 |
| 40  | NA    | 92/94 (98%)   | 92 (100%)  | 0        | 100         | 100 |
| 41  | OA    | 74/75 (99%)   | 73 (99%)   | 1 (1%)   | 59          | 76  |
| 42  | PA    | 108/121 (89%) | 107 (99%)  | 1 (1%)   | 70          | 80  |
| 43  | RA    | 126/137 (92%) | 117 (93%)  | 9 (7%)   | 13          | 41  |

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 52  | AB    | 180/244 (74%)  | 179 (99%)  | 1 (1%)   | 78          | 83  |
| 53  | BB    | 194/231 (84%)  | 192 (99%)  | 2 (1%)   | 68          | 79  |
| 54  | CB    | 186/225 (83%)  | 185 (100%) | 1 (0%)   | 81          | 85  |
| 55  | DB    | 190/232 (82%)  | 189 (100%) | 1 (0%)   | 81          | 85  |
| 56  | EB    | 224/225 (100%) | 219 (98%)  | 5 (2%)   | 45          | 71  |
| 57  | FB    | 158/170 (93%)  | 156 (99%)  | 2 (1%)   | 61          | 77  |
| 58  | GB    | 207/218 (95%)  | 203 (98%)  | 4 (2%)   | 50          | 73  |
| 59  | HB    | 165/360 (46%)  | 161 (98%)  | 4 (2%)   | 43          | 69  |
| 60  | IB    | 178/180 (99%)  | 176 (99%)  | 2 (1%)   | 65          | 78  |
| 61  | JB    | 161/168 (96%)  | 160 (99%)  | 1 (1%)   | 78          | 83  |
| 62  | KB    | 87/136 (64%)   | 86 (99%)   | 1 (1%)   | 65          | 78  |
| 63  | LB    | 130/142 (92%)  | 128 (98%)  | 2 (2%)   | 57          | 75  |
| 64  | MB    | 99/108 (92%)   | 93 (94%)   | 6 (6%)   | 17          | 46  |
| 65  | NB    | 130/131 (99%)  | 129 (99%)  | 1 (1%)   | 73          | 81  |
| 66  | OB    | 106/119 (89%)  | 105 (99%)  | 1 (1%)   | 70          | 80  |
| 67  | PB    | 115/130 (88%)  | 111 (96%)  | 4 (4%)   | 32          | 62  |
| 68  | QB    | 117/140 (84%)  | 114 (97%)  | 3 (3%)   | 40          | 68  |
| 69  | RB    | 119/121 (98%)  | 115 (97%)  | 4 (3%)   | 32          | 63  |
| 70  | SB    | 125/132 (95%)  | 123 (98%)  | 2 (2%)   | 55          | 75  |
| 71  | TB    | 112/115 (97%)  | 109 (97%)  | 3 (3%)   | 39          | 67  |
| 72  | UB    | 93/107 (87%)   | 90 (97%)   | 3 (3%)   | 34          | 64  |
| 73  | VB    | 67/67 (100%)   | 66 (98%)   | 1 (2%)   | 57          | 75  |
| 74  | WB    | 112/113 (99%)  | 111 (99%)  | 1 (1%)   | 70          | 80  |
| 75  | XB    | 113/115 (98%)  | 110 (97%)  | 3 (3%)   | 39          | 67  |
| 76  | YB    | 107/113 (95%)  | 107 (100%) | 0        | 100         | 100 |
| 77  | ZB    | 75/102 (74%)   | 74 (99%)   | 1 (1%)   | 61          | 77  |
| 78  | AC    | 88/98 (90%)    | 87 (99%)   | 1 (1%)   | 65          | 78  |
| 79  | BC    | 75/76 (99%)    | 73 (97%)   | 2 (3%)   | 39          | 67  |
| 80  | CC    | 55/62 (89%)    | 55 (100%)  | 0        | 100         | 100 |
| 81  | DC    | 48/49 (98%)    | 47 (98%)   | 1 (2%)   | 47          | 71  |
| 82  | EC    | 46/106 (43%)   | 44 (96%)   | 2 (4%)   | 26          | 57  |

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| Mol | Chain | Analysed          | Rotameric   | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|----------|-------------|-----|
| 83  | FC    | 62/154 (40%)      | 59 (95%)    | 3 (5%)   | 23          | 54  |
| 84  | GC    | 272/275 (99%)     | 252 (93%)   | 20 (7%)  | 13          | 40  |
| 86  | b     | 138/258 (54%)     | 128 (93%)   | 10 (7%)  | 13          | 40  |
| 87  | c     | 12/12 (100%)      | 12 (100%)   | 0        | 100         | 100 |
| 88  | HC    | 179/379 (47%)     | 163 (91%)   | 16 (9%)  | 9           | 33  |
| All | All   | 10256/12074 (85%) | 10069 (98%) | 187 (2%) | 51          | 73  |

All (187) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 32  | VAL  |
| 2   | B     | 162 | VAL  |
| 2   | B     | 248 | LEU  |
| 2   | B     | 258 | HIS  |
| 2   | B     | 298 | LEU  |
| 2   | B     | 314 | ILE  |
| 2   | B     | 338 | VAL  |
| 2   | B     | 353 | VAL  |
| 3   | C     | 115 | VAL  |
| 3   | C     | 232 | VAL  |
| 4   | D     | 163 | LEU  |
| 5   | E     | 178 | VAL  |
| 5   | E     | 189 | LEU  |
| 7   | G     | 159 | THR  |
| 7   | G     | 193 | VAL  |
| 7   | G     | 221 | VAL  |
| 8   | H     | 47  | LEU  |
| 8   | H     | 73  | ILE  |
| 8   | H     | 95  | VAL  |
| 8   | H     | 123 | ILE  |
| 9   | I     | 126 | VAL  |
| 9   | I     | 184 | MET  |
| 10  | J     | 87  | LEU  |
| 10  | J     | 129 | ASP  |
| 11  | K     | 63  | THR  |
| 11  | K     | 64  | VAL  |
| 11  | K     | 70  | VAL  |
| 11  | K     | 90  | VAL  |
| 13  | M     | 60  | VAL  |
| 13  | M     | 64  | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13  | M     | 142 | ILE  |
| 13  | M     | 184 | ILE  |
| 16  | P     | 22  | ASP  |
| 16  | P     | 83  | VAL  |
| 18  | R     | 84  | TYR  |
| 18  | R     | 132 | ILE  |
| 18  | R     | 154 | LEU  |
| 18  | R     | 160 | ARG  |
| 19  | S     | 80  | VAL  |
| 19  | S     | 143 | THR  |
| 21  | U     | 92  | ASP  |
| 21  | U     | 109 | LYS  |
| 22  | V     | 87  | LEU  |
| 23  | W     | 52  | LEU  |
| 24  | X     | 79  | VAL  |
| 24  | X     | 82  | ILE  |
| 24  | X     | 95  | VAL  |
| 24  | X     | 104 | VAL  |
| 25  | Y     | 53  | VAL  |
| 26  | Z     | 122 | VAL  |
| 28  | BA    | 14  | ILE  |
| 28  | BA    | 71  | VAL  |
| 30  | DA    | 107 | ASN  |
| 32  | FA    | 22  | LEU  |
| 32  | FA    | 32  | TYR  |
| 32  | FA    | 67  | LEU  |
| 33  | GA    | 17  | LEU  |
| 33  | GA    | 96  | ASN  |
| 33  | GA    | 116 | LEU  |
| 35  | IA    | 59  | THR  |
| 37  | KA    | 51  | LEU  |
| 38  | LA    | 100 | LYS  |
| 41  | OA    | 52  | VAL  |
| 42  | PA    | 103 | HIS  |
| 43  | RA    | 13  | VAL  |
| 43  | RA    | 37  | LEU  |
| 43  | RA    | 58  | ILE  |
| 43  | RA    | 66  | ASN  |
| 43  | RA    | 92  | ARG  |
| 43  | RA    | 137 | GLN  |
| 43  | RA    | 147 | HIS  |
| 43  | RA    | 151 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 43  | RA    | 154 | ASP  |
| 52  | AB    | 124 | VAL  |
| 53  | BB    | 82  | ARG  |
| 53  | BB    | 126 | ASP  |
| 54  | CB    | 248 | TYR  |
| 55  | DB    | 205 | TYR  |
| 56  | EB    | 12  | VAL  |
| 56  | EB    | 62  | LYS  |
| 56  | EB    | 207 | VAL  |
| 56  | EB    | 220 | THR  |
| 56  | EB    | 222 | LEU  |
| 57  | FB    | 102 | LEU  |
| 57  | FB    | 109 | LEU  |
| 58  | GB    | 50  | VAL  |
| 58  | GB    | 153 | VAL  |
| 58  | GB    | 157 | VAL  |
| 58  | GB    | 213 | LEU  |
| 59  | HB    | 284 | THR  |
| 59  | HB    | 313 | ILE  |
| 59  | HB    | 372 | VAL  |
| 59  | HB    | 405 | GLU  |
| 60  | IB    | 107 | THR  |
| 60  | IB    | 125 | LYS  |
| 61  | JB    | 66  | LYS  |
| 62  | KB    | 47  | LYS  |
| 63  | LB    | 48  | LYS  |
| 63  | LB    | 52  | GLU  |
| 64  | MB    | 27  | ILE  |
| 64  | MB    | 28  | HIS  |
| 64  | MB    | 31  | LEU  |
| 64  | MB    | 57  | ASP  |
| 64  | MB    | 62  | VAL  |
| 64  | MB    | 111 | VAL  |
| 65  | NB    | 54  | LEU  |
| 66  | OB    | 56  | VAL  |
| 67  | PB    | 37  | TYR  |
| 67  | PB    | 65  | LYS  |
| 67  | PB    | 72  | LYS  |
| 67  | PB    | 90  | VAL  |
| 68  | QB    | 75  | TYR  |
| 68  | QB    | 110 | ILE  |
| 68  | QB    | 126 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 69  | RB    | 6   | THR  |
| 69  | RB    | 95  | ILE  |
| 69  | RB    | 99  | ASP  |
| 69  | RB    | 132 | ARG  |
| 70  | SB    | 3   | LEU  |
| 70  | SB    | 131 | VAL  |
| 71  | TB    | 4   | VAL  |
| 71  | TB    | 24  | LYS  |
| 71  | TB    | 99  | VAL  |
| 72  | UB    | 17  | ILE  |
| 72  | UB    | 18  | HIS  |
| 72  | UB    | 68  | THR  |
| 73  | VB    | 11  | LEU  |
| 74  | WB    | 105 | THR  |
| 75  | XB    | 17  | ARG  |
| 75  | XB    | 81  | ILE  |
| 75  | XB    | 105 | PHE  |
| 77  | ZB    | 32  | LYS  |
| 78  | AC    | 100 | ARG  |
| 79  | BC    | 43  | ILE  |
| 79  | BC    | 80  | ARG  |
| 81  | DC    | 39  | CYS  |
| 82  | EC    | 118 | VAL  |
| 82  | EC    | 124 | LYS  |
| 83  | FC    | 85  | TYR  |
| 83  | FC    | 108 | VAL  |
| 83  | FC    | 135 | HIS  |
| 84  | GC    | 8   | ARG  |
| 84  | GC    | 11  | LEU  |
| 84  | GC    | 18  | VAL  |
| 84  | GC    | 31  | ILE  |
| 84  | GC    | 38  | LYS  |
| 84  | GC    | 54  | ILE  |
| 84  | GC    | 68  | ASP  |
| 84  | GC    | 113 | PHE  |
| 84  | GC    | 120 | ILE  |
| 84  | GC    | 141 | THR  |
| 84  | GC    | 142 | VAL  |
| 84  | GC    | 164 | ILE  |
| 84  | GC    | 177 | TRP  |
| 84  | GC    | 186 | THR  |
| 84  | GC    | 198 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 84  | GC    | 256 | ILE  |
| 84  | GC    | 274 | VAL  |
| 84  | GC    | 275 | ILE  |
| 84  | GC    | 280 | LYS  |
| 84  | GC    | 297 | THR  |
| 86  | b     | 21  | LEU  |
| 86  | b     | 53  | VAL  |
| 86  | b     | 54  | LEU  |
| 86  | b     | 69  | LEU  |
| 86  | b     | 75  | LEU  |
| 86  | b     | 105 | ASN  |
| 86  | b     | 116 | ILE  |
| 86  | b     | 149 | ARG  |
| 86  | b     | 219 | VAL  |
| 86  | b     | 222 | VAL  |
| 88  | HC    | 240 | ARG  |
| 88  | HC    | 248 | LEU  |
| 88  | HC    | 287 | THR  |
| 88  | HC    | 290 | LYS  |
| 88  | HC    | 312 | VAL  |
| 88  | HC    | 313 | LYS  |
| 88  | HC    | 347 | LEU  |
| 88  | HC    | 360 | VAL  |
| 88  | HC    | 371 | LYS  |
| 88  | HC    | 387 | LEU  |
| 88  | HC    | 408 | LYS  |
| 88  | HC    | 429 | MET  |
| 88  | HC    | 432 | THR  |
| 88  | HC    | 438 | ILE  |
| 88  | HC    | 439 | LYS  |
| 88  | HC    | 444 | LYS  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (88) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 205 | ASN  |
| 3   | C     | 21  | ASN  |
| 3   | C     | 41  | HIS  |
| 3   | C     | 187 | GLN  |
| 3   | C     | 203 | GLN  |
| 3   | C     | 329 | ASN  |
| 3   | C     | 347 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | D     | 131 | ASN  |
| 4   | D     | 275 | GLN  |
| 4   | D     | 282 | GLN  |
| 6   | F     | 98  | ASN  |
| 8   | H     | 63  | ASN  |
| 9   | I     | 59  | GLN  |
| 9   | I     | 73  | ASN  |
| 10  | J     | 23  | ASN  |
| 11  | K     | 159 | ASN  |
| 12  | L     | 48  | GLN  |
| 12  | L     | 125 | ASN  |
| 13  | M     | 182 | HIS  |
| 15  | O     | 10  | ASN  |
| 15  | O     | 93  | ASN  |
| 17  | Q     | 34  | ASN  |
| 17  | Q     | 58  | HIS  |
| 17  | Q     | 118 | HIS  |
| 18  | R     | 163 | HIS  |
| 19  | S     | 127 | GLN  |
| 19  | S     | 139 | HIS  |
| 20  | T     | 38  | ASN  |
| 20  | T     | 105 | ASN  |
| 21  | U     | 108 | ASN  |
| 22  | V     | 48  | GLN  |
| 27  | AA    | 6   | ASN  |
| 28  | BA    | 33  | GLN  |
| 28  | BA    | 72  | HIS  |
| 29  | CA    | 18  | ASN  |
| 29  | CA    | 116 | ASN  |
| 31  | EA    | 55  | ASN  |
| 32  | FA    | 14  | ASN  |
| 34  | HA    | 15  | HIS  |
| 35  | IA    | 48  | ASN  |
| 37  | KA    | 33  | ASN  |
| 42  | PA    | 21  | ASN  |
| 42  | PA    | 31  | ASN  |
| 42  | PA    | 100 | ASN  |
| 43  | RA    | 137 | GLN  |
| 53  | BB    | 158 | HIS  |
| 53  | BB    | 186 | ASN  |
| 53  | BB    | 202 | GLN  |
| 54  | CB    | 136 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 54  | CB    | 172 | ASN  |
| 54  | CB    | 178 | HIS  |
| 55  | DB    | 95  | ASN  |
| 56  | EB    | 50  | ASN  |
| 57  | FB    | 79  | HIS  |
| 58  | GB    | 110 | ASN  |
| 59  | HB    | 271 | ASN  |
| 60  | IB    | 7   | ASN  |
| 60  | IB    | 22  | HIS  |
| 60  | IB    | 35  | ASN  |
| 60  | IB    | 155 | ASN  |
| 61  | JB    | 124 | HIS  |
| 61  | JB    | 140 | GLN  |
| 63  | LB    | 19  | ASN  |
| 64  | MB    | 46  | GLN  |
| 64  | MB    | 75  | ASN  |
| 65  | NB    | 49  | GLN  |
| 65  | NB    | 58  | HIS  |
| 66  | OB    | 32  | HIS  |
| 68  | QB    | 37  | GLN  |
| 68  | QB    | 55  | ASN  |
| 69  | RB    | 116 | ASN  |
| 70  | SB    | 10  | GLN  |
| 71  | TB    | 126 | GLN  |
| 73  | VB    | 21  | ASN  |
| 74  | WB    | 15  | ASN  |
| 75  | XB    | 61  | GLN  |
| 76  | YB    | 29  | HIS  |
| 76  | YB    | 63  | HIS  |
| 76  | YB    | 112 | ASN  |
| 77  | ZB    | 112 | ASN  |
| 78  | AC    | 7   | ASN  |
| 80  | CC    | 29  | GLN  |
| 80  | CC    | 45  | ASN  |
| 81  | DC    | 16  | GLN  |
| 84  | GC    | 222 | ASN  |
| 86  | b     | 42  | GLN  |
| 88  | HC    | 348 | ASN  |
| 88  | HC    | 367 | HIS  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 44  | SA    | 75/76 (98%)     | 16 (21%)          | 3 (4%)          |
| 45  | TA    | 75/76 (98%)     | 16 (21%)          | 0               |
| 46  | UA    | 74/75 (98%)     | 38 (51%)          | 1 (1%)          |
| 47  | VA    | 11/12 (91%)     | 3 (27%)           | 0               |
| 48  | WA    | 3556/3584 (99%) | 610 (17%)         | 20 (0%)         |
| 49  | XA    | 118/120 (98%)   | 10 (8%)           | 0               |
| 50  | YA    | 155/156 (99%)   | 32 (20%)          | 0               |
| 51  | ZA    | 1707/1869 (91%) | 327 (19%)         | 9 (0%)          |
| All | All   | 5771/5968 (96%) | 1052 (18%)        | 33 (0%)         |

All (1052) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 44  | SA    | 9   | A    |
| 44  | SA    | 16  | C    |
| 44  | SA    | 18  | G    |
| 44  | SA    | 19  | C    |
| 44  | SA    | 20  | A    |
| 44  | SA    | 21  | A    |
| 44  | SA    | 22  | A    |
| 44  | SA    | 46  | G    |
| 44  | SA    | 47  | U    |
| 44  | SA    | 48  | C    |
| 44  | SA    | 49  | C    |
| 44  | SA    | 58  | A    |
| 44  | SA    | 60  | A    |
| 44  | SA    | 61  | C    |
| 44  | SA    | 70  | A    |
| 44  | SA    | 76  | A    |
| 45  | TA    | 6   | G    |
| 45  | TA    | 7   | A    |
| 45  | TA    | 10  | G    |
| 45  | TA    | 13  | C    |
| 45  | TA    | 16  | C    |
| 45  | TA    | 17  | U    |
| 45  | TA    | 18  | G    |
| 45  | TA    | 19  | A    |
| 45  | TA    | 20  | U    |
| 45  | TA    | 22  | G    |
| 45  | TA    | 31  | A    |
| 45  | TA    | 34  | U    |
| 45  | TA    | 35  | U    |
| 45  | TA    | 47  | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 45  | TA    | 58  | A    |
| 45  | TA    | 76  | A    |
| 46  | UA    | 8   | U    |
| 46  | UA    | 16  | C    |
| 46  | UA    | 17  | G    |
| 46  | UA    | 18  | G    |
| 46  | UA    | 19  | U    |
| 46  | UA    | 20  | U    |
| 46  | UA    | 21  | A    |
| 46  | UA    | 22  | U    |
| 46  | UA    | 24  | A    |
| 46  | UA    | 25  | C    |
| 46  | UA    | 26  | G    |
| 46  | UA    | 30  | G    |
| 46  | UA    | 31  | C    |
| 46  | UA    | 32  | C    |
| 46  | UA    | 33  | U    |
| 46  | UA    | 34  | U    |
| 46  | UA    | 38  | C    |
| 46  | UA    | 40  | C    |
| 46  | UA    | 41  | G    |
| 46  | UA    | 42  | A    |
| 46  | UA    | 43  | A    |
| 46  | UA    | 44  | A    |
| 46  | UA    | 46  | G    |
| 46  | UA    | 48  | C    |
| 46  | UA    | 49  | C    |
| 46  | UA    | 52  | G    |
| 46  | UA    | 56  | C    |
| 46  | UA    | 58  | A    |
| 46  | UA    | 59  | A    |
| 46  | UA    | 60  | A    |
| 46  | UA    | 61  | C    |
| 46  | UA    | 66  | C    |
| 46  | UA    | 67  | G    |
| 46  | UA    | 70  | A    |
| 46  | UA    | 71  | A    |
| 46  | UA    | 74  | C    |
| 46  | UA    | 75  | C    |
| 46  | UA    | 76  | A    |
| 47  | VA    | 22  | U    |
| 47  | VA    | 24  | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 47  | VA    | 26  | A    |
| 48  | WA    | 12  | A    |
| 48  | WA    | 13  | U    |
| 48  | WA    | 25  | A    |
| 48  | WA    | 39  | A    |
| 48  | WA    | 42  | A    |
| 48  | WA    | 48  | G    |
| 48  | WA    | 56  | A    |
| 48  | WA    | 59  | A    |
| 48  | WA    | 64  | A    |
| 48  | WA    | 65  | A    |
| 48  | WA    | 66  | A    |
| 48  | WA    | 91  | G    |
| 48  | WA    | 109 | G    |
| 48  | WA    | 110 | C    |
| 48  | WA    | 117 | C    |
| 48  | WA    | 119 | G    |
| 48  | WA    | 120 | A    |
| 48  | WA    | 130 | C    |
| 48  | WA    | 132 | G    |
| 48  | WA    | 133 | C    |
| 48  | WA    | 134 | G    |
| 48  | WA    | 135 | G    |
| 48  | WA    | 136 | C    |
| 48  | WA    | 138 | G    |
| 48  | WA    | 142 | G    |
| 48  | WA    | 143 | C    |
| 48  | WA    | 144 | G    |
| 48  | WA    | 151 | G    |
| 48  | WA    | 157 | U    |
| 48  | WA    | 159 | C    |
| 48  | WA    | 169 | A    |
| 48  | WA    | 171 | U    |
| 48  | WA    | 172 | C    |
| 48  | WA    | 173 | C    |
| 48  | WA    | 179 | G    |
| 48  | WA    | 182 | G    |
| 48  | WA    | 197 | A    |
| 48  | WA    | 200 | U    |
| 48  | WA    | 201 | C    |
| 48  | WA    | 209 | U    |
| 48  | WA    | 217 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 48  | WA    | 218 | A    |
| 48  | WA    | 219 | G    |
| 48  | WA    | 220 | C    |
| 48  | WA    | 224 | U    |
| 48  | WA    | 233 | U    |
| 48  | WA    | 234 | G    |
| 48  | WA    | 253 | G    |
| 48  | WA    | 263 | G    |
| 48  | WA    | 266 | C    |
| 48  | WA    | 267 | G    |
| 48  | WA    | 276 | C    |
| 48  | WA    | 280 | G    |
| 48  | WA    | 297 | U    |
| 48  | WA    | 306 | A    |
| 48  | WA    | 315 | G    |
| 48  | WA    | 316 | U    |
| 48  | WA    | 334 | A    |
| 48  | WA    | 340 | C    |
| 48  | WA    | 350 | C    |
| 48  | WA    | 363 | A    |
| 48  | WA    | 373 | G    |
| 48  | WA    | 379 | G    |
| 48  | WA    | 386 | A    |
| 48  | WA    | 387 | G    |
| 48  | WA    | 399 | G    |
| 48  | WA    | 409 | G    |
| 48  | WA    | 410 | A    |
| 48  | WA    | 412 | G    |
| 48  | WA    | 414 | C    |
| 48  | WA    | 449 | C    |
| 48  | WA    | 450 | G    |
| 48  | WA    | 452 | A    |
| 48  | WA    | 454 | U    |
| 48  | WA    | 455 | C    |
| 48  | WA    | 467 | U    |
| 48  | WA    | 468 | U    |
| 48  | WA    | 482 | C    |
| 48  | WA    | 483 | G    |
| 48  | WA    | 484 | G    |
| 48  | WA    | 485 | U    |
| 48  | WA    | 487 | C    |
| 48  | WA    | 488 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 48  | WA    | 489 | G    |
| 48  | WA    | 493 | U    |
| 48  | WA    | 494 | G    |
| 48  | WA    | 499 | C    |
| 48  | WA    | 500 | G    |
| 48  | WA    | 506 | G    |
| 48  | WA    | 511 | U    |
| 48  | WA    | 521 | U    |
| 48  | WA    | 662 | C    |
| 48  | WA    | 667 | G    |
| 48  | WA    | 686 | C    |
| 48  | WA    | 697 | C    |
| 48  | WA    | 698 | G    |
| 48  | WA    | 705 | C    |
| 48  | WA    | 720 | C    |
| 48  | WA    | 732 | G    |
| 48  | WA    | 739 | C    |
| 48  | WA    | 741 | G    |
| 48  | WA    | 751 | G    |
| 48  | WA    | 761 | G    |
| 48  | WA    | 905 | U    |
| 48  | WA    | 907 | C    |
| 48  | WA    | 915 | U    |
| 48  | WA    | 917 | A    |
| 48  | WA    | 919 | A    |
| 48  | WA    | 920 | G    |
| 48  | WA    | 929 | C    |
| 48  | WA    | 930 | G    |
| 48  | WA    | 933 | A    |
| 48  | WA    | 936 | A    |
| 48  | WA    | 937 | G    |
| 48  | WA    | 938 | C    |
| 48  | WA    | 939 | A    |
| 48  | WA    | 940 | G    |
| 48  | WA    | 941 | C    |
| 48  | WA    | 944 | G    |
| 48  | WA    | 946 | C    |
| 48  | WA    | 949 | A    |
| 48  | WA    | 950 | U    |
| 48  | WA    | 964 | G    |
| 48  | WA    | 965 | A    |
| 48  | WA    | 966 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 48  | WA    | 971  | A    |
| 48  | WA    | 972  | C    |
| 48  | WA    | 974  | C    |
| 48  | WA    | 978  | C    |
| 48  | WA    | 989  | C    |
| 48  | WA    | 1078 | C    |
| 48  | WA    | 1084 | A    |
| 48  | WA    | 1085 | C    |
| 48  | WA    | 1102 | C    |
| 48  | WA    | 1103 | C    |
| 48  | WA    | 1104 | G    |
| 48  | WA    | 1186 | C    |
| 48  | WA    | 1200 | G    |
| 48  | WA    | 1201 | G    |
| 48  | WA    | 1202 | G    |
| 48  | WA    | 1206 | G    |
| 48  | WA    | 1208 | C    |
| 48  | WA    | 1216 | C    |
| 48  | WA    | 1217 | G    |
| 48  | WA    | 1221 | C    |
| 48  | WA    | 1222 | C    |
| 48  | WA    | 1240 | G    |
| 48  | WA    | 1243 | C    |
| 48  | WA    | 1244 | A    |
| 48  | WA    | 1246 | G    |
| 48  | WA    | 1253 | C    |
| 48  | WA    | 1255 | G    |
| 48  | WA    | 1258 | A    |
| 48  | WA    | 1259 | A    |
| 48  | WA    | 1265 | A    |
| 48  | WA    | 1270 | G    |
| 48  | WA    | 1271 | G    |
| 48  | WA    | 1272 | A    |
| 48  | WA    | 1274 | C    |
| 48  | WA    | 1275 | G    |
| 48  | WA    | 1282 | C    |
| 48  | WA    | 1286 | G    |
| 48  | WA    | 1287 | U    |
| 48  | WA    | 1289 | G    |
| 48  | WA    | 1290 | G    |
| 48  | WA    | 1294 | C    |
| 48  | WA    | 1298 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 48  | WA    | 1303 | C    |
| 48  | WA    | 1305 | A    |
| 48  | WA    | 1328 | A    |
| 48  | WA    | 1356 | A    |
| 48  | WA    | 1360 | G    |
| 48  | WA    | 1361 | G    |
| 48  | WA    | 1379 | G    |
| 48  | WA    | 1381 | C    |
| 48  | WA    | 1382 | G    |
| 48  | WA    | 1383 | U    |
| 48  | WA    | 1389 | A    |
| 48  | WA    | 1396 | G    |
| 48  | WA    | 1399 | A    |
| 48  | WA    | 1400 | A    |
| 48  | WA    | 1421 | G    |
| 48  | WA    | 1422 | A    |
| 48  | WA    | 1435 | A    |
| 48  | WA    | 1447 | U    |
| 48  | WA    | 1448 | C    |
| 48  | WA    | 1459 | G    |
| 48  | WA    | 1485 | C    |
| 48  | WA    | 1499 | A    |
| 48  | WA    | 1500 | G    |
| 48  | WA    | 1503 | C    |
| 48  | WA    | 1504 | G    |
| 48  | WA    | 1520 | A    |
| 48  | WA    | 1525 | A    |
| 48  | WA    | 1527 | A    |
| 48  | WA    | 1536 | A    |
| 48  | WA    | 1549 | A    |
| 48  | WA    | 1566 | A    |
| 48  | WA    | 1568 | C    |
| 48  | WA    | 1580 | U    |
| 48  | WA    | 1593 | U    |
| 48  | WA    | 1598 | U    |
| 48  | WA    | 1599 | G    |
| 48  | WA    | 1604 | U    |
| 48  | WA    | 1614 | G    |
| 48  | WA    | 1626 | G    |
| 48  | WA    | 1627 | G    |
| 48  | WA    | 1633 | A    |
| 48  | WA    | 1635 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 48  | WA    | 1636 | A    |
| 48  | WA    | 1640 | A    |
| 48  | WA    | 1643 | G    |
| 48  | WA    | 1656 | G    |
| 48  | WA    | 1663 | C    |
| 48  | WA    | 1678 | C    |
| 48  | WA    | 1679 | U    |
| 48  | WA    | 1686 | A    |
| 48  | WA    | 1693 | G    |
| 48  | WA    | 1743 | G    |
| 48  | WA    | 1744 | A    |
| 48  | WA    | 1748 | A    |
| 48  | WA    | 1756 | U    |
| 48  | WA    | 1757 | C    |
| 48  | WA    | 1763 | G    |
| 48  | WA    | 1765 | C    |
| 48  | WA    | 1768 | A    |
| 48  | WA    | 1769 | A    |
| 48  | WA    | 1770 | C    |
| 48  | WA    | 1771 | G    |
| 48  | WA    | 1772 | A    |
| 48  | WA    | 1774 | C    |
| 48  | WA    | 1782 | A    |
| 48  | WA    | 1783 | U    |
| 48  | WA    | 1789 | A    |
| 48  | WA    | 1806 | A    |
| 48  | WA    | 1807 | A    |
| 48  | WA    | 1817 | G    |
| 48  | WA    | 1821 | G    |
| 48  | WA    | 1823 | G    |
| 48  | WA    | 1824 | U    |
| 48  | WA    | 1830 | C    |
| 48  | WA    | 1836 | U    |
| 48  | WA    | 1838 | G    |
| 48  | WA    | 1839 | A    |
| 48  | WA    | 1844 | G    |
| 48  | WA    | 1857 | G    |
| 48  | WA    | 1871 | G    |
| 48  | WA    | 1880 | G    |
| 48  | WA    | 1890 | A    |
| 48  | WA    | 1899 | A    |
| 48  | WA    | 1912 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 48  | WA    | 1920 | U    |
| 48  | WA    | 1922 | C    |
| 48  | WA    | 1923 | C    |
| 48  | WA    | 1924 | G    |
| 48  | WA    | 1931 | A    |
| 48  | WA    | 1933 | C    |
| 48  | WA    | 1950 | G    |
| 48  | WA    | 1963 | G    |
| 48  | WA    | 1964 | A    |
| 48  | WA    | 1975 | G    |
| 48  | WA    | 1976 | U    |
| 48  | WA    | 1977 | G    |
| 48  | WA    | 1984 | G    |
| 48  | WA    | 1985 | A    |
| 48  | WA    | 1986 | A    |
| 48  | WA    | 1987 | G    |
| 48  | WA    | 1988 | U    |
| 48  | WA    | 1989 | C    |
| 48  | WA    | 1990 | G    |
| 48  | WA    | 1992 | A    |
| 48  | WA    | 1993 | A    |
| 48  | WA    | 1999 | U    |
| 48  | WA    | 2000 | A    |
| 48  | WA    | 2003 | G    |
| 48  | WA    | 2004 | A    |
| 48  | WA    | 2005 | G    |
| 48  | WA    | 2010 | U    |
| 48  | WA    | 2023 | G    |
| 48  | WA    | 2027 | A    |
| 48  | WA    | 2028 | A    |
| 48  | WA    | 2046 | U    |
| 48  | WA    | 2048 | G    |
| 48  | WA    | 2049 | A    |
| 48  | WA    | 2050 | U    |
| 48  | WA    | 2054 | G    |
| 48  | WA    | 2057 | G    |
| 48  | WA    | 2058 | G    |
| 48  | WA    | 2064 | C    |
| 48  | WA    | 2071 | A    |
| 48  | WA    | 2086 | U    |
| 48  | WA    | 2095 | G    |
| 48  | WA    | 2096 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 48  | WA    | 2097 | A    |
| 48  | WA    | 2099 | A    |
| 48  | WA    | 2102 | G    |
| 48  | WA    | 2104 | G    |
| 48  | WA    | 2106 | A    |
| 48  | WA    | 2107 | A    |
| 48  | WA    | 2108 | G    |
| 48  | WA    | 2109 | A    |
| 48  | WA    | 2114 | G    |
| 48  | WA    | 2118 | C    |
| 48  | WA    | 2261 | G    |
| 48  | WA    | 2262 | C    |
| 48  | WA    | 2269 | U    |
| 48  | WA    | 2270 | A    |
| 48  | WA    | 2277 | G    |
| 48  | WA    | 2291 | C    |
| 48  | WA    | 2302 | A    |
| 48  | WA    | 2303 | G    |
| 48  | WA    | 2308 | G    |
| 48  | WA    | 2315 | A    |
| 48  | WA    | 2316 | G    |
| 48  | WA    | 2333 | G    |
| 48  | WA    | 2335 | G    |
| 48  | WA    | 2350 | G    |
| 48  | WA    | 2353 | C    |
| 48  | WA    | 2362 | A    |
| 48  | WA    | 2384 | A    |
| 48  | WA    | 2397 | A    |
| 48  | WA    | 2412 | C    |
| 48  | WA    | 2419 | A    |
| 48  | WA    | 2424 | C    |
| 48  | WA    | 2427 | U    |
| 48  | WA    | 2434 | U    |
| 48  | WA    | 2435 | G    |
| 48  | WA    | 2436 | G    |
| 48  | WA    | 2473 | G    |
| 48  | WA    | 2477 | G    |
| 48  | WA    | 2485 | G    |
| 48  | WA    | 2491 | C    |
| 48  | WA    | 2492 | U    |
| 48  | WA    | 2493 | C    |
| 48  | WA    | 2505 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 48  | WA    | 2506 | C    |
| 48  | WA    | 2507 | C    |
| 48  | WA    | 2509 | A    |
| 48  | WA    | 2515 | A    |
| 48  | WA    | 2531 | A    |
| 48  | WA    | 2539 | A    |
| 48  | WA    | 2546 | G    |
| 48  | WA    | 2547 | U    |
| 48  | WA    | 2548 | G    |
| 48  | WA    | 2549 | G    |
| 48  | WA    | 2555 | A    |
| 48  | WA    | 2585 | C    |
| 48  | WA    | 2588 | G    |
| 48  | WA    | 2591 | C    |
| 48  | WA    | 2603 | A    |
| 48  | WA    | 2620 | G    |
| 48  | WA    | 2622 | G    |
| 48  | WA    | 2629 | C    |
| 48  | WA    | 2640 | G    |
| 48  | WA    | 2655 | C    |
| 48  | WA    | 2664 | G    |
| 48  | WA    | 2672 | C    |
| 48  | WA    | 2677 | G    |
| 48  | WA    | 2688 | G    |
| 48  | WA    | 2689 | U    |
| 48  | WA    | 2697 | A    |
| 48  | WA    | 2698 | A    |
| 48  | WA    | 2705 | G    |
| 48  | WA    | 2707 | G    |
| 48  | WA    | 2709 | U    |
| 48  | WA    | 2710 | U    |
| 48  | WA    | 2711 | C    |
| 48  | WA    | 2712 | C    |
| 48  | WA    | 2713 | G    |
| 48  | WA    | 2721 | C    |
| 48  | WA    | 2723 | G    |
| 48  | WA    | 2727 | A    |
| 48  | WA    | 2728 | G    |
| 48  | WA    | 2742 | U    |
| 48  | WA    | 2756 | G    |
| 48  | WA    | 2760 | G    |
| 48  | WA    | 2766 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 48  | WA    | 2771 | U    |
| 48  | WA    | 2789 | A    |
| 48  | WA    | 2790 | U    |
| 48  | WA    | 2792 | U    |
| 48  | WA    | 2796 | C    |
| 48  | WA    | 2800 | A    |
| 48  | WA    | 2808 | A    |
| 48  | WA    | 2816 | C    |
| 48  | WA    | 2828 | U    |
| 48  | WA    | 2829 | G    |
| 48  | WA    | 2830 | U    |
| 48  | WA    | 2845 | U    |
| 48  | WA    | 2857 | G    |
| 48  | WA    | 2899 | G    |
| 48  | WA    | 3599 | G    |
| 48  | WA    | 3600 | C    |
| 48  | WA    | 3617 | G    |
| 48  | WA    | 3627 | G    |
| 48  | WA    | 3628 | G    |
| 48  | WA    | 3637 | A    |
| 48  | WA    | 3650 | A    |
| 48  | WA    | 3664 | A    |
| 48  | WA    | 3666 | G    |
| 48  | WA    | 3674 | G    |
| 48  | WA    | 3714 | A    |
| 48  | WA    | 3716 | G    |
| 48  | WA    | 3750 | A    |
| 48  | WA    | 3755 | G    |
| 48  | WA    | 3763 | C    |
| 48  | WA    | 3774 | U    |
| 48  | WA    | 3775 | U    |
| 48  | WA    | 3776 | A    |
| 48  | WA    | 3778 | G    |
| 48  | WA    | 3779 | G    |
| 48  | WA    | 3786 | A    |
| 48  | WA    | 3788 | U    |
| 48  | WA    | 3800 | U    |
| 48  | WA    | 3804 | U    |
| 48  | WA    | 3812 | C    |
| 48  | WA    | 3813 | G    |
| 48  | WA    | 3816 | U    |
| 48  | WA    | 3819 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 48  | WA    | 3821 | G    |
| 48  | WA    | 3840 | U    |
| 48  | WA    | 3841 | G    |
| 48  | WA    | 3842 | U    |
| 48  | WA    | 3871 | C    |
| 48  | WA    | 3878 | A    |
| 48  | WA    | 3879 | A    |
| 48  | WA    | 3880 | C    |
| 48  | WA    | 3881 | G    |
| 48  | WA    | 3891 | G    |
| 48  | WA    | 3894 | U    |
| 48  | WA    | 3899 | G    |
| 48  | WA    | 3903 | A    |
| 48  | WA    | 3908 | A    |
| 48  | WA    | 3909 | G    |
| 48  | WA    | 3910 | A    |
| 48  | WA    | 3916 | U    |
| 48  | WA    | 3917 | U    |
| 48  | WA    | 3919 | A    |
| 48  | WA    | 3940 | G    |
| 48  | WA    | 3941 | G    |
| 48  | WA    | 3945 | A    |
| 48  | WA    | 3949 | A    |
| 48  | WA    | 3951 | A    |
| 48  | WA    | 3953 | G    |
| 48  | WA    | 4066 | C    |
| 48  | WA    | 4078 | G    |
| 48  | WA    | 4088 | G    |
| 48  | WA    | 4090 | C    |
| 48  | WA    | 4097 | G    |
| 48  | WA    | 4100 | A    |
| 48  | WA    | 4101 | G    |
| 48  | WA    | 4118 | C    |
| 48  | WA    | 4121 | C    |
| 48  | WA    | 4123 | G    |
| 48  | WA    | 4124 | G    |
| 48  | WA    | 4129 | A    |
| 48  | WA    | 4130 | A    |
| 48  | WA    | 4136 | C    |
| 48  | WA    | 4137 | G    |
| 48  | WA    | 4141 | G    |
| 48  | WA    | 4143 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 48  | WA    | 4144 | C    |
| 48  | WA    | 4145 | C    |
| 48  | WA    | 4146 | G    |
| 48  | WA    | 4160 | C    |
| 48  | WA    | 4164 | C    |
| 48  | WA    | 4168 | G    |
| 48  | WA    | 4172 | A    |
| 48  | WA    | 4174 | A    |
| 48  | WA    | 4175 | G    |
| 48  | WA    | 4185 | G    |
| 48  | WA    | 4186 | G    |
| 48  | WA    | 4193 | G    |
| 48  | WA    | 4205 | A    |
| 48  | WA    | 4214 | A    |
| 48  | WA    | 4231 | U    |
| 48  | WA    | 4235 | A    |
| 48  | WA    | 4236 | A    |
| 48  | WA    | 4253 | A    |
| 48  | WA    | 4256 | G    |
| 48  | WA    | 4268 | G    |
| 48  | WA    | 4270 | A    |
| 48  | WA    | 4273 | A    |
| 48  | WA    | 4275 | A    |
| 48  | WA    | 4283 | A    |
| 48  | WA    | 4293 | G    |
| 48  | WA    | 4299 | G    |
| 48  | WA    | 4306 | A    |
| 48  | WA    | 4307 | G    |
| 48  | WA    | 4308 | U    |
| 48  | WA    | 4316 | C    |
| 48  | WA    | 4332 | G    |
| 48  | WA    | 4334 | C    |
| 48  | WA    | 4351 | C    |
| 48  | WA    | 4352 | C    |
| 48  | WA    | 4356 | U    |
| 48  | WA    | 4375 | G    |
| 48  | WA    | 4379 | G    |
| 48  | WA    | 4380 | A    |
| 48  | WA    | 4382 | A    |
| 48  | WA    | 4389 | C    |
| 48  | WA    | 4396 | A    |
| 48  | WA    | 4397 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 48  | WA    | 4398 | A    |
| 48  | WA    | 4421 | U    |
| 48  | WA    | 4423 | C    |
| 48  | WA    | 4424 | A    |
| 48  | WA    | 4439 | U    |
| 48  | WA    | 4446 | C    |
| 48  | WA    | 4450 | G    |
| 48  | WA    | 4451 | A    |
| 48  | WA    | 4454 | U    |
| 48  | WA    | 4455 | C    |
| 48  | WA    | 4466 | A    |
| 48  | WA    | 4468 | C    |
| 48  | WA    | 4502 | U    |
| 48  | WA    | 4514 | U    |
| 48  | WA    | 4515 | A    |
| 48  | WA    | 4520 | A    |
| 48  | WA    | 4522 | G    |
| 48  | WA    | 4524 | G    |
| 48  | WA    | 4526 | G    |
| 48  | WA    | 4531 | G    |
| 48  | WA    | 4532 | U    |
| 48  | WA    | 4533 | U    |
| 48  | WA    | 4550 | A    |
| 48  | WA    | 4551 | G    |
| 48  | WA    | 4562 | C    |
| 48  | WA    | 4569 | G    |
| 48  | WA    | 4575 | G    |
| 48  | WA    | 4577 | G    |
| 48  | WA    | 4579 | U    |
| 48  | WA    | 4583 | G    |
| 48  | WA    | 4588 | G    |
| 48  | WA    | 4592 | A    |
| 48  | WA    | 4602 | G    |
| 48  | WA    | 4629 | U    |
| 48  | WA    | 4638 | U    |
| 48  | WA    | 4639 | G    |
| 48  | WA    | 4654 | G    |
| 48  | WA    | 4658 | A    |
| 48  | WA    | 4669 | C    |
| 48  | WA    | 4672 | C    |
| 48  | WA    | 4674 | A    |
| 48  | WA    | 4679 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 48  | WA    | 4693 | A    |
| 48  | WA    | 4702 | A    |
| 48  | WA    | 4711 | U    |
| 48  | WA    | 4722 | C    |
| 48  | WA    | 4723 | G    |
| 48  | WA    | 4747 | G    |
| 48  | WA    | 4756 | G    |
| 48  | WA    | 4759 | C    |
| 48  | WA    | 4761 | C    |
| 48  | WA    | 4763 | G    |
| 48  | WA    | 4767 | G    |
| 48  | WA    | 4771 | G    |
| 48  | WA    | 4772 | U    |
| 48  | WA    | 4779 | C    |
| 48  | WA    | 4872 | G    |
| 48  | WA    | 4873 | C    |
| 48  | WA    | 4875 | G    |
| 48  | WA    | 4876 | A    |
| 48  | WA    | 4877 | G    |
| 48  | WA    | 4878 | A    |
| 48  | WA    | 4879 | G    |
| 48  | WA    | 4884 | U    |
| 48  | WA    | 4885 | C    |
| 48  | WA    | 4887 | U    |
| 48  | WA    | 4888 | C    |
| 48  | WA    | 4906 | G    |
| 48  | WA    | 4912 | A    |
| 48  | WA    | 4914 | G    |
| 48  | WA    | 4917 | G    |
| 48  | WA    | 4919 | C    |
| 48  | WA    | 4923 | C    |
| 48  | WA    | 4924 | C    |
| 48  | WA    | 4926 | C    |
| 48  | WA    | 4927 | U    |
| 48  | WA    | 4928 | C    |
| 48  | WA    | 4929 | G    |
| 48  | WA    | 4930 | C    |
| 48  | WA    | 4936 | A    |
| 48  | WA    | 4939 | C    |
| 48  | WA    | 4945 | A    |
| 48  | WA    | 4946 | C    |
| 48  | WA    | 4949 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 48  | WA    | 4951 | G    |
| 48  | WA    | 4952 | U    |
| 48  | WA    | 4953 | G    |
| 48  | WA    | 4960 | C    |
| 48  | WA    | 4965 | G    |
| 48  | WA    | 4967 | U    |
| 48  | WA    | 4968 | A    |
| 48  | WA    | 4978 | U    |
| 48  | WA    | 4981 | A    |
| 48  | WA    | 4992 | C    |
| 48  | WA    | 4993 | U    |
| 48  | WA    | 4994 | G    |
| 48  | WA    | 5008 | U    |
| 48  | WA    | 5016 | A    |
| 48  | WA    | 5019 | G    |
| 48  | WA    | 5043 | G    |
| 48  | WA    | 5049 | C    |
| 48  | WA    | 5050 | A    |
| 48  | WA    | 5052 | C    |
| 48  | WA    | 5055 | U    |
| 48  | WA    | 5056 | C    |
| 48  | WA    | 5063 | A    |
| 48  | WA    | 5064 | G    |
| 49  | XA    | 7    | G    |
| 49  | XA    | 11   | A    |
| 49  | XA    | 33   | U    |
| 49  | XA    | 41   | G    |
| 49  | XA    | 50   | A    |
| 49  | XA    | 54   | A    |
| 49  | XA    | 63   | C    |
| 49  | XA    | 64   | G    |
| 49  | XA    | 100  | A    |
| 49  | XA    | 110  | G    |
| 50  | YA    | 34   | U    |
| 50  | YA    | 35   | C    |
| 50  | YA    | 39   | G    |
| 50  | YA    | 59   | A    |
| 50  | YA    | 62   | A    |
| 50  | YA    | 63   | U    |
| 50  | YA    | 72   | A    |
| 50  | YA    | 75   | G    |
| 50  | YA    | 79   | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 50  | YA    | 80  | A    |
| 50  | YA    | 81  | C    |
| 50  | YA    | 82  | A    |
| 50  | YA    | 83  | C    |
| 50  | YA    | 84  | A    |
| 50  | YA    | 85  | U    |
| 50  | YA    | 86  | U    |
| 50  | YA    | 87  | G    |
| 50  | YA    | 90  | C    |
| 50  | YA    | 94  | G    |
| 50  | YA    | 95  | A    |
| 50  | YA    | 103 | A    |
| 50  | YA    | 105 | C    |
| 50  | YA    | 110 | U    |
| 50  | YA    | 111 | U    |
| 50  | YA    | 112 | G    |
| 50  | YA    | 114 | G    |
| 50  | YA    | 123 | U    |
| 50  | YA    | 124 | U    |
| 50  | YA    | 125 | C    |
| 50  | YA    | 126 | C    |
| 50  | YA    | 127 | U    |
| 50  | YA    | 150 | C    |
| 51  | ZA    | 3   | C    |
| 51  | ZA    | 25  | A    |
| 51  | ZA    | 33  | G    |
| 51  | ZA    | 41  | G    |
| 51  | ZA    | 42  | A    |
| 51  | ZA    | 44  | U    |
| 51  | ZA    | 46  | A    |
| 51  | ZA    | 56  | G    |
| 51  | ZA    | 58  | C    |
| 51  | ZA    | 65  | C    |
| 51  | ZA    | 67  | C    |
| 51  | ZA    | 68  | A    |
| 51  | ZA    | 71  | G    |
| 51  | ZA    | 73  | C    |
| 51  | ZA    | 75  | G    |
| 51  | ZA    | 76  | U    |
| 51  | ZA    | 79  | A    |
| 51  | ZA    | 82  | G    |
| 51  | ZA    | 103 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 51  | ZA    | 113 | G    |
| 51  | ZA    | 114 | G    |
| 51  | ZA    | 115 | U    |
| 51  | ZA    | 116 | U    |
| 51  | ZA    | 126 | G    |
| 51  | ZA    | 130 | G    |
| 51  | ZA    | 142 | C    |
| 51  | ZA    | 143 | U    |
| 51  | ZA    | 147 | A    |
| 51  | ZA    | 155 | G    |
| 51  | ZA    | 160 | U    |
| 51  | ZA    | 162 | C    |
| 51  | ZA    | 173 | A    |
| 51  | ZA    | 178 | C    |
| 51  | ZA    | 181 | A    |
| 51  | ZA    | 182 | C    |
| 51  | ZA    | 183 | G    |
| 51  | ZA    | 184 | G    |
| 51  | ZA    | 187 | G    |
| 51  | ZA    | 188 | C    |
| 51  | ZA    | 192 | C    |
| 51  | ZA    | 199 | C    |
| 51  | ZA    | 200 | G    |
| 51  | ZA    | 201 | C    |
| 51  | ZA    | 204 | G    |
| 51  | ZA    | 209 | A    |
| 51  | ZA    | 291 | G    |
| 51  | ZA    | 292 | A    |
| 51  | ZA    | 306 | C    |
| 51  | ZA    | 307 | G    |
| 51  | ZA    | 308 | G    |
| 51  | ZA    | 309 | G    |
| 51  | ZA    | 320 | G    |
| 51  | ZA    | 322 | C    |
| 51  | ZA    | 323 | C    |
| 51  | ZA    | 325 | C    |
| 51  | ZA    | 326 | C    |
| 51  | ZA    | 327 | G    |
| 51  | ZA    | 328 | U    |
| 51  | ZA    | 329 | G    |
| 51  | ZA    | 334 | C    |
| 51  | ZA    | 335 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 51  | ZA    | 347 | G    |
| 51  | ZA    | 351 | G    |
| 51  | ZA    | 362 | C    |
| 51  | ZA    | 364 | A    |
| 51  | ZA    | 368 | U    |
| 51  | ZA    | 369 | C    |
| 51  | ZA    | 371 | A    |
| 51  | ZA    | 383 | G    |
| 51  | ZA    | 385 | G    |
| 51  | ZA    | 386 | C    |
| 51  | ZA    | 400 | C    |
| 51  | ZA    | 409 | C    |
| 51  | ZA    | 418 | A    |
| 51  | ZA    | 438 | G    |
| 51  | ZA    | 448 | A    |
| 51  | ZA    | 450 | C    |
| 51  | ZA    | 464 | A    |
| 51  | ZA    | 472 | C    |
| 51  | ZA    | 473 | A    |
| 51  | ZA    | 474 | G    |
| 51  | ZA    | 482 | G    |
| 51  | ZA    | 487 | U    |
| 51  | ZA    | 492 | C    |
| 51  | ZA    | 493 | A    |
| 51  | ZA    | 508 | A    |
| 51  | ZA    | 525 | A    |
| 51  | ZA    | 531 | A    |
| 51  | ZA    | 532 | C    |
| 51  | ZA    | 534 | G    |
| 51  | ZA    | 535 | G    |
| 51  | ZA    | 538 | U    |
| 51  | ZA    | 539 | C    |
| 51  | ZA    | 541 | U    |
| 51  | ZA    | 542 | U    |
| 51  | ZA    | 544 | G    |
| 51  | ZA    | 545 | A    |
| 51  | ZA    | 547 | G    |
| 51  | ZA    | 548 | C    |
| 51  | ZA    | 549 | C    |
| 51  | ZA    | 550 | C    |
| 51  | ZA    | 554 | A    |
| 51  | ZA    | 555 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 51  | ZA    | 559 | G    |
| 51  | ZA    | 560 | A    |
| 51  | ZA    | 561 | A    |
| 51  | ZA    | 562 | U    |
| 51  | ZA    | 563 | G    |
| 51  | ZA    | 564 | A    |
| 51  | ZA    | 568 | C    |
| 51  | ZA    | 574 | A    |
| 51  | ZA    | 576 | A    |
| 51  | ZA    | 582 | U    |
| 51  | ZA    | 583 | A    |
| 51  | ZA    | 587 | A    |
| 51  | ZA    | 588 | G    |
| 51  | ZA    | 590 | A    |
| 51  | ZA    | 591 | U    |
| 51  | ZA    | 593 | C    |
| 51  | ZA    | 594 | A    |
| 51  | ZA    | 606 | G    |
| 51  | ZA    | 608 | C    |
| 51  | ZA    | 614 | C    |
| 51  | ZA    | 617 | G    |
| 51  | ZA    | 626 | G    |
| 51  | ZA    | 627 | U    |
| 51  | ZA    | 631 | U    |
| 51  | ZA    | 643 | A    |
| 51  | ZA    | 644 | G    |
| 51  | ZA    | 660 | C    |
| 51  | ZA    | 668 | A    |
| 51  | ZA    | 669 | A    |
| 51  | ZA    | 671 | A    |
| 51  | ZA    | 672 | A    |
| 51  | ZA    | 673 | G    |
| 51  | ZA    | 684 | G    |
| 51  | ZA    | 689 | U    |
| 51  | ZA    | 752 | G    |
| 51  | ZA    | 753 | C    |
| 51  | ZA    | 754 | G    |
| 51  | ZA    | 798 | G    |
| 51  | ZA    | 799 | U    |
| 51  | ZA    | 811 | A    |
| 51  | ZA    | 812 | A    |
| 51  | ZA    | 821 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 51  | ZA    | 822  | U    |
| 51  | ZA    | 834  | C    |
| 51  | ZA    | 835  | C    |
| 51  | ZA    | 840  | C    |
| 51  | ZA    | 841  | G    |
| 51  | ZA    | 845  | G    |
| 51  | ZA    | 847  | A    |
| 51  | ZA    | 859  | G    |
| 51  | ZA    | 860  | G    |
| 51  | ZA    | 869  | A    |
| 51  | ZA    | 870  | A    |
| 51  | ZA    | 871  | U    |
| 51  | ZA    | 872  | A    |
| 51  | ZA    | 873  | G    |
| 51  | ZA    | 874  | G    |
| 51  | ZA    | 875  | A    |
| 51  | ZA    | 878  | G    |
| 51  | ZA    | 886  | A    |
| 51  | ZA    | 888  | U    |
| 51  | ZA    | 889  | U    |
| 51  | ZA    | 890  | U    |
| 51  | ZA    | 891  | G    |
| 51  | ZA    | 892  | U    |
| 51  | ZA    | 897  | U    |
| 51  | ZA    | 898  | U    |
| 51  | ZA    | 902  | G    |
| 51  | ZA    | 905  | C    |
| 51  | ZA    | 913  | A    |
| 51  | ZA    | 914  | U    |
| 51  | ZA    | 920  | A    |
| 51  | ZA    | 922  | A    |
| 51  | ZA    | 933  | G    |
| 51  | ZA    | 934  | G    |
| 51  | ZA    | 956  | G    |
| 51  | ZA    | 971  | G    |
| 51  | ZA    | 985  | G    |
| 51  | ZA    | 990  | A    |
| 51  | ZA    | 992  | A    |
| 51  | ZA    | 999  | G    |
| 51  | ZA    | 1002 | U    |
| 51  | ZA    | 1008 | A    |
| 51  | ZA    | 1023 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 51  | ZA    | 1061 | U    |
| 51  | ZA    | 1062 | A    |
| 51  | ZA    | 1078 | C    |
| 51  | ZA    | 1083 | A    |
| 51  | ZA    | 1085 | C    |
| 51  | ZA    | 1115 | U    |
| 51  | ZA    | 1116 | C    |
| 51  | ZA    | 1117 | C    |
| 51  | ZA    | 1118 | C    |
| 51  | ZA    | 1121 | G    |
| 51  | ZA    | 1126 | G    |
| 51  | ZA    | 1133 | A    |
| 51  | ZA    | 1138 | C    |
| 51  | ZA    | 1148 | A    |
| 51  | ZA    | 1149 | A    |
| 51  | ZA    | 1153 | C    |
| 51  | ZA    | 1154 | U    |
| 51  | ZA    | 1195 | A    |
| 51  | ZA    | 1207 | G    |
| 51  | ZA    | 1208 | A    |
| 51  | ZA    | 1215 | C    |
| 51  | ZA    | 1224 | G    |
| 51  | ZA    | 1227 | G    |
| 51  | ZA    | 1233 | G    |
| 51  | ZA    | 1241 | A    |
| 51  | ZA    | 1242 | U    |
| 51  | ZA    | 1251 | A    |
| 51  | ZA    | 1253 | A    |
| 51  | ZA    | 1256 | G    |
| 51  | ZA    | 1257 | G    |
| 51  | ZA    | 1259 | A    |
| 51  | ZA    | 1260 | A    |
| 51  | ZA    | 1274 | G    |
| 51  | ZA    | 1275 | G    |
| 51  | ZA    | 1285 | G    |
| 51  | ZA    | 1286 | G    |
| 51  | ZA    | 1297 | U    |
| 51  | ZA    | 1298 | G    |
| 51  | ZA    | 1299 | A    |
| 51  | ZA    | 1300 | U    |
| 51  | ZA    | 1301 | A    |
| 51  | ZA    | 1302 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 51  | ZA    | 1303 | C    |
| 51  | ZA    | 1313 | A    |
| 51  | ZA    | 1333 | U    |
| 51  | ZA    | 1342 | U    |
| 51  | ZA    | 1354 | G    |
| 51  | ZA    | 1371 | U    |
| 51  | ZA    | 1372 | U    |
| 51  | ZA    | 1378 | A    |
| 51  | ZA    | 1382 | A    |
| 51  | ZA    | 1396 | A    |
| 51  | ZA    | 1397 | U    |
| 51  | ZA    | 1404 | U    |
| 51  | ZA    | 1417 | C    |
| 51  | ZA    | 1418 | C    |
| 51  | ZA    | 1419 | C    |
| 51  | ZA    | 1420 | G    |
| 51  | ZA    | 1421 | A    |
| 51  | ZA    | 1422 | G    |
| 51  | ZA    | 1423 | C    |
| 51  | ZA    | 1424 | G    |
| 51  | ZA    | 1428 | G    |
| 51  | ZA    | 1433 | C    |
| 51  | ZA    | 1434 | C    |
| 51  | ZA    | 1435 | C    |
| 51  | ZA    | 1437 | C    |
| 51  | ZA    | 1438 | A    |
| 51  | ZA    | 1439 | A    |
| 51  | ZA    | 1441 | U    |
| 51  | ZA    | 1442 | U    |
| 51  | ZA    | 1452 | A    |
| 51  | ZA    | 1454 | A    |
| 51  | ZA    | 1464 | C    |
| 51  | ZA    | 1466 | G    |
| 51  | ZA    | 1475 | G    |
| 51  | ZA    | 1476 | A    |
| 51  | ZA    | 1477 | U    |
| 51  | ZA    | 1489 | A    |
| 51  | ZA    | 1490 | G    |
| 51  | ZA    | 1498 | A    |
| 51  | ZA    | 1521 | C    |
| 51  | ZA    | 1522 | A    |
| 51  | ZA    | 1531 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 51  | ZA    | 1533 | A    |
| 51  | ZA    | 1535 | U    |
| 51  | ZA    | 1536 | G    |
| 51  | ZA    | 1548 | G    |
| 51  | ZA    | 1551 | U    |
| 51  | ZA    | 1552 | G    |
| 51  | ZA    | 1553 | C    |
| 51  | ZA    | 1555 | U    |
| 51  | ZA    | 1556 | A    |
| 51  | ZA    | 1560 | U    |
| 51  | ZA    | 1564 | C    |
| 51  | ZA    | 1567 | G    |
| 51  | ZA    | 1580 | A    |
| 51  | ZA    | 1585 | U    |
| 51  | ZA    | 1587 | G    |
| 51  | ZA    | 1588 | A    |
| 51  | ZA    | 1601 | A    |
| 51  | ZA    | 1604 | G    |
| 51  | ZA    | 1605 | G    |
| 51  | ZA    | 1606 | G    |
| 51  | ZA    | 1621 | U    |
| 51  | ZA    | 1623 | A    |
| 51  | ZA    | 1638 | G    |
| 51  | ZA    | 1646 | C    |
| 51  | ZA    | 1648 | G    |
| 51  | ZA    | 1665 | G    |
| 51  | ZA    | 1680 | G    |
| 51  | ZA    | 1683 | C    |
| 51  | ZA    | 1698 | C    |
| 51  | ZA    | 1699 | A    |
| 51  | ZA    | 1721 | U    |
| 51  | ZA    | 1722 | G    |
| 51  | ZA    | 1726 | G    |
| 51  | ZA    | 1744 | G    |
| 51  | ZA    | 1745 | A    |
| 51  | ZA    | 1748 | G    |
| 51  | ZA    | 1753 | C    |
| 51  | ZA    | 1757 | G    |
| 51  | ZA    | 1774 | C    |
| 51  | ZA    | 1775 | U    |
| 51  | ZA    | 1776 | G    |
| 51  | ZA    | 1780 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 51  | ZA    | 1783 | C    |
| 51  | ZA    | 1824 | A    |
| 51  | ZA    | 1825 | A    |
| 51  | ZA    | 1826 | G    |
| 51  | ZA    | 1831 | A    |
| 51  | ZA    | 1836 | G    |
| 51  | ZA    | 1838 | U    |
| 51  | ZA    | 1849 | G    |
| 51  | ZA    | 1851 | A    |
| 51  | ZA    | 1861 | G    |
| 51  | ZA    | 1862 | G    |
| 51  | ZA    | 1863 | A    |
| 51  | ZA    | 1865 | C    |
| 51  | ZA    | 1869 | A    |

All (33) RNA pucker outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 44  | SA    | 20   | A    |
| 44  | SA    | 21   | A    |
| 44  | SA    | 57   | G    |
| 46  | UA    | 19   | U    |
| 48  | WA    | 12   | A    |
| 48  | WA    | 275  | C    |
| 48  | WA    | 385  | A    |
| 48  | WA    | 505  | G    |
| 48  | WA    | 971  | A    |
| 48  | WA    | 1293 | G    |
| 48  | WA    | 1635 | G    |
| 48  | WA    | 1677 | C    |
| 48  | WA    | 1806 | A    |
| 48  | WA    | 1820 | G    |
| 48  | WA    | 2048 | G    |
| 48  | WA    | 2095 | G    |
| 48  | WA    | 2268 | C    |
| 48  | WA    | 2697 | A    |
| 48  | WA    | 3627 | G    |
| 48  | WA    | 4117 | G    |
| 48  | WA    | 4450 | G    |
| 48  | WA    | 4701 | U    |
| 48  | WA    | 4886 | G    |
| 48  | WA    | 4951 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 51  | ZA    | 24   | C    |
| 51  | ZA    | 370  | G    |
| 51  | ZA    | 541  | U    |
| 51  | ZA    | 561  | A    |
| 51  | ZA    | 752  | G    |
| 51  | ZA    | 870  | A    |
| 51  | ZA    | 890  | U    |
| 51  | ZA    | 1137 | U    |
| 51  | ZA    | 1433 | C    |

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 219 ligands modelled in this entry, 213 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res  | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |      |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 93  | SPD  | WA    | 5229 | -    | 9,9,9        | 0.28 | 0           | 8,8,8       | 0.33 | 0           |
| 93  | SPD  | WA    | 5230 | -    | 9,9,9        | 0.28 | 0           | 8,8,8       | 0.29 | 0           |
| 93  | SPD  | ZA    | 1933 | -    | 9,9,9        | 0.26 | 0           | 8,8,8       | 0.30 | 0           |
| 91  | 5GP  | UA    | 101  | 46   | 26,26,26     | 0.98 | 1 (3%)      | 39,40,40    | 1.77 | 7 (17%)     |
| 95  | SER  | HC    | 502  | -    | 4,5,6        | 0.57 | 0           | 1,5,7       | 0.58 | 0           |
| 92  | ANM  | WA    | 5228 | 94   | 20,20,20     | 4.08 | 7 (35%)     | 24,27,27    | 1.38 | 2 (8%)      |

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   |
|-----|------|-------|------|------|---------|------------|---------|
| 93  | SPD  | WA    | 5229 | -    | -       | 0/7/7/7    | -       |
| 93  | SPD  | WA    | 5230 | -    | -       | 1/7/7/7    | -       |
| 93  | SPD  | ZA    | 1933 | -    | -       | 1/7/7/7    | -       |
| 91  | 5GP  | UA    | 101  | 46   | -       | 5/10/26/26 | 0/3/3/3 |
| 95  | SER  | HC    | 502  | -    | -       | 0/2/4/6    | -       |
| 92  | ANM  | WA    | 5228 | 94   | -       | 6/10/23/23 | 0/2/2/2 |

All (8) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms  | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|--------|-------------|----------|
| 92  | WA    | 5228 | ANM  | C3-C2  | -11.79 | 1.32        | 1.53     |
| 92  | WA    | 5228 | ANM  | C16-N1 | -8.89  | 1.30        | 1.47     |
| 92  | WA    | 5228 | ANM  | C2-C16 | 7.41   | 1.68        | 1.53     |
| 92  | WA    | 5228 | ANM  | C4-C3  | 3.97   | 1.58        | 1.53     |
| 92  | WA    | 5228 | ANM  | C4-N1  | 3.86   | 1.60        | 1.47     |
| 92  | WA    | 5228 | ANM  | O2-C5  | 3.52   | 1.43        | 1.35     |
| 91  | UA    | 101  | 5GP  | C6-N1  | -2.47  | 1.34        | 1.38     |
| 92  | WA    | 5228 | ANM  | C6-C5  | 2.44   | 1.57        | 1.49     |

All (9) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 91  | UA    | 101  | 5GP  | C5-C4-N3 | -6.03 | 118.79      | 128.39   |
| 92  | WA    | 5228 | ANM  | O2-C5-C6 | 5.04  | 120.08      | 111.09   |
| 91  | UA    | 101  | 5GP  | C2-N3-C4 | 4.75  | 120.49      | 112.30   |
| 91  | UA    | 101  | 5GP  | N9-C4-N3 | 3.85  | 133.66      | 125.95   |
| 91  | UA    | 101  | 5GP  | C5-C6-N1 | 2.48  | 119.57      | 113.25   |
| 91  | UA    | 101  | 5GP  | O6-C6-C5 | -2.36 | 120.31      | 126.53   |
| 91  | UA    | 101  | 5GP  | C2-N1-C6 | -2.34 | 120.88      | 125.11   |
| 92  | WA    | 5228 | ANM  | C2-O2-C5 | -2.28 | 114.17      | 117.72   |
| 91  | UA    | 101  | 5GP  | N9-C8-N7 | -2.22 | 109.29      | 113.40   |

There are no chirality outliers.

All (13) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms        |
|-----|-------|------|------|--------------|
| 92  | WA    | 5228 | ANM  | C6-C5-O2-C2  |
| 92  | WA    | 5228 | ANM  | O3-C5-O2-C2  |
| 92  | WA    | 5228 | ANM  | C1-C9-O1-C14 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 92  | WA    | 5228 | ANM  | C10-C9-O1-C14   |
| 91  | UA    | 101  | 5GP  | O4'-C4'-C5'-O5' |
| 91  | UA    | 101  | 5GP  | C3'-C4'-C5'-O5' |
| 93  | WA    | 5230 | SPD  | C8-C7-N6-C5     |
| 91  | UA    | 101  | 5GP  | C5'-O5'-P-OP1   |
| 93  | ZA    | 1933 | SPD  | C2-C3-C4-C5     |
| 92  | WA    | 5228 | ANM  | C11-C12-C15-C16 |
| 92  | WA    | 5228 | ANM  | C13-C12-C15-C16 |
| 91  | UA    | 101  | 5GP  | C4'-C5'-O5'-P   |
| 91  | UA    | 101  | 5GP  | C5'-O5'-P-OP2   |

There are no ring outliers.

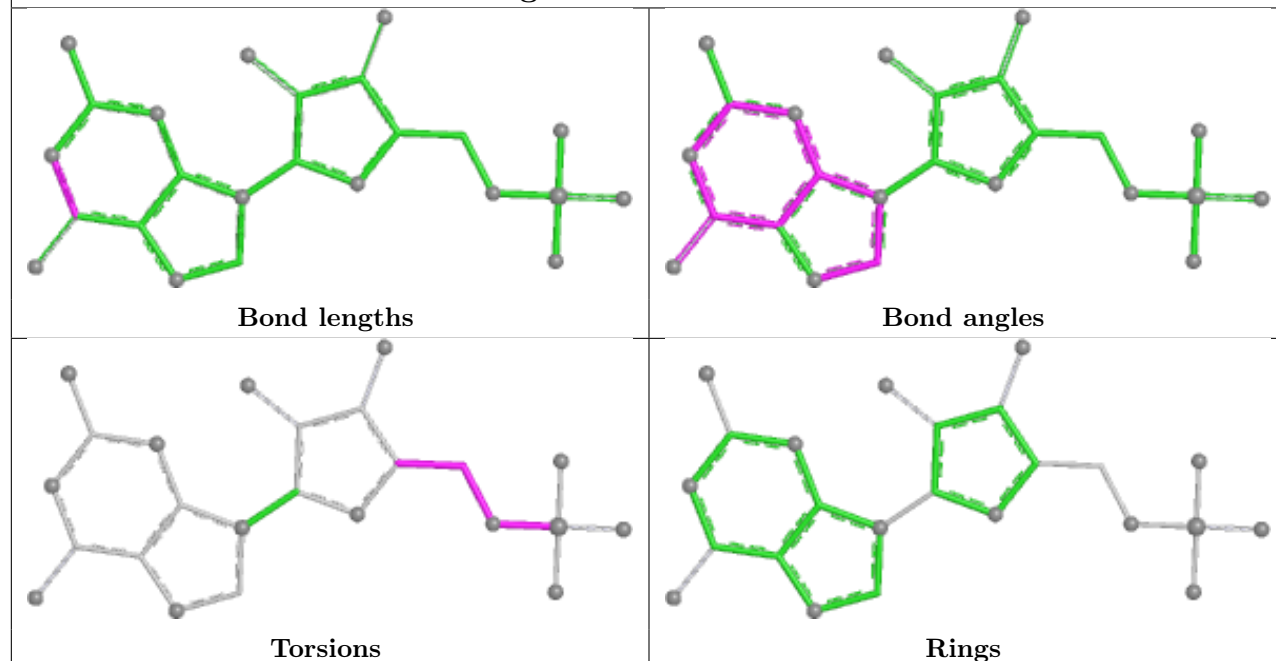
2 monomers are involved in 2 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 93  | WA    | 5229 | SPD  | 1       | 0            |
| 92  | WA    | 5228 | ANM  | 1       | 0            |

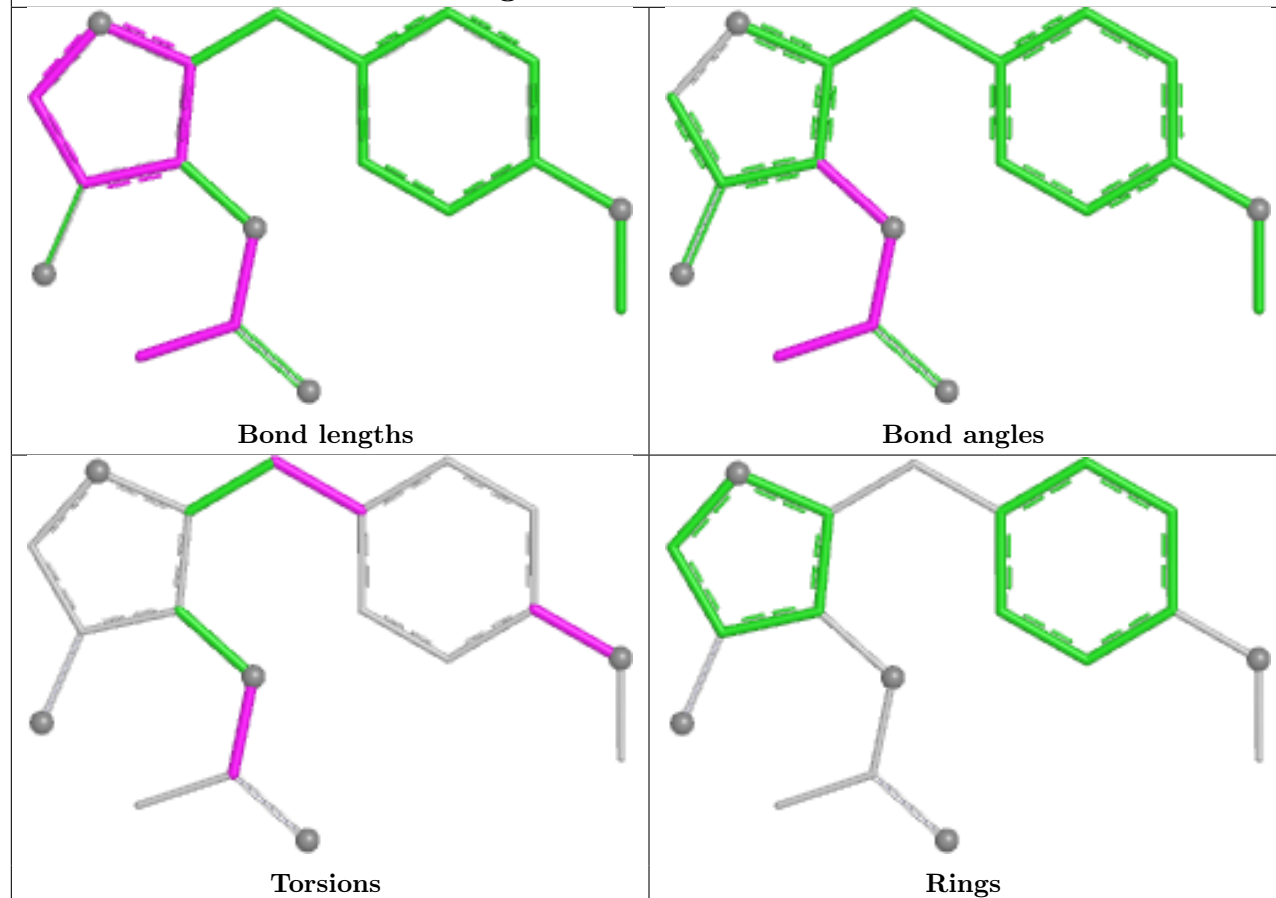
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



## Ligand 5GP UA 101



## Ligand ANM WA 5228



## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 48  | WA    | 21               |
| 86  | b     | 2                |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | WA    | 2118:C    | O3'    | 2260:C    | P      | 37.14        |
| 1     | WA    | 1225:G    | O3'    | 1239:G    | P      | 20.72        |
| 1     | WA    | 996:C     | O3'    | 1070:G    | P      | 17.81        |
| 1     | WA    | 4779:C    | O3'    | 4861:C    | P      | 17.44        |
| 1     | WA    | 524:C     | O3'    | 639:G     | P      | 16.85        |
| 1     | WA    | 763:G     | O3'    | 904:C     | P      | 16.83        |
| 1     | WA    | 4103:C    | O3'    | 4109:G    | P      | 16.58        |
| 1     | WA    | 1698:C    | O3'    | 1722:C    | P      | 14.92        |
| 1     | WA    | 5024:U    | O3'    | 5030:G    | P      | 13.93        |
| 1     | WA    | 1366:U    | O3'    | 1370:A    | P      | 13.62        |
| 1     | WA    | 2904:G    | O3'    | 3598:A    | P      | 12.69        |
| 1     | b     | 106:LYS   | C      | 107:VAL   | N      | 11.91        |
| 1     | WA    | 4731:A    | O3'    | 4737:G    | P      | 10.44        |
| 1     | WA    | 3954:A    | O3'    | 4063:C    | P      | 10.11        |
| 1     | WA    | 1186:C    | O3'    | 1189:C    | P      | 9.75         |
| 1     | WA    | 182:G     | O3'    | 189:G     | P      | 9.42         |
| 1     | b     | 107:VAL   | C      | 108:PRO   | N      | 8.67         |
| 1     | WA    | 513:U     | O3'    | 516:C     | P      | 5.66         |
| 1     | WA    | 4742:G    | O3'    | 4745:G    | P      | 5.66         |
| 1     | WA    | 501:G     | O3'    | 505:G     | P      | 4.99         |
| 1     | WA    | 1106:U    | O3'    | 1174:G    | P      | 4.39         |
| 1     | WA    | 4901:G    | O3'    | 4904:C    | P      | 4.35         |
| 1     | WA    | 2030:C    | O3'    | 2031:A    | P      | 3.62         |

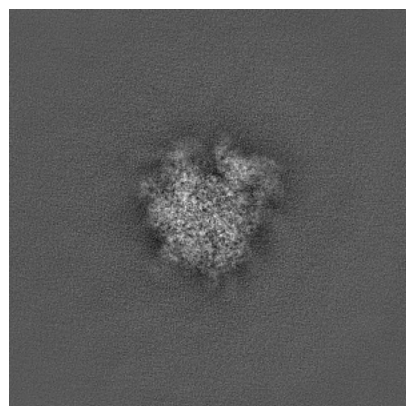
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-43566. These allow visual inspection of the internal detail of the map and identification of artifacts.

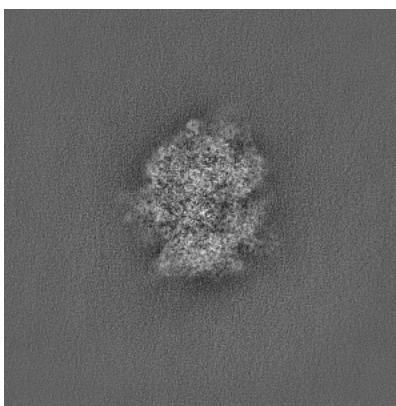
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

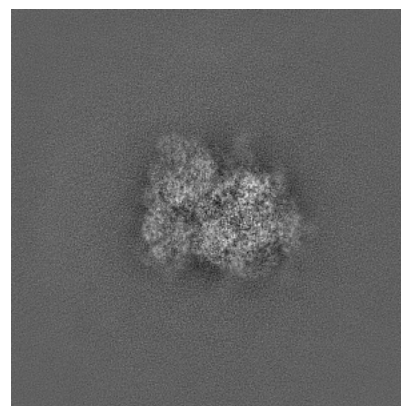
#### 6.1.1 Primary map



X

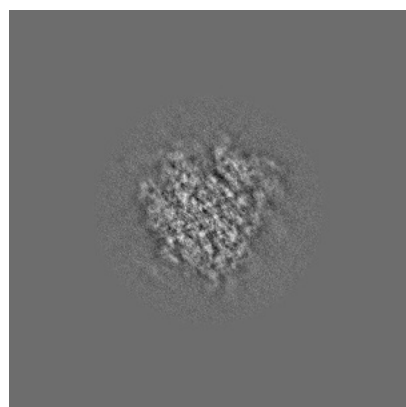


Y

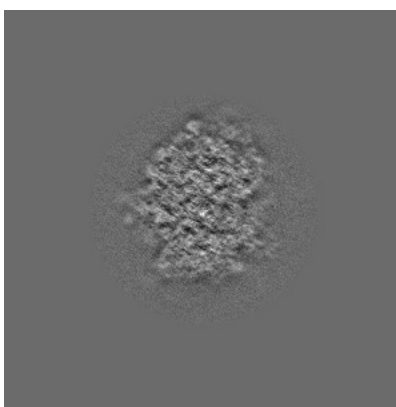


Z

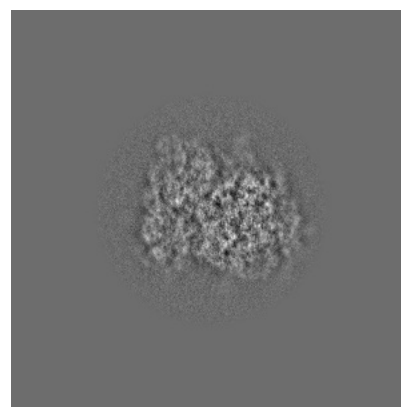
#### 6.1.2 Raw map



X



Y

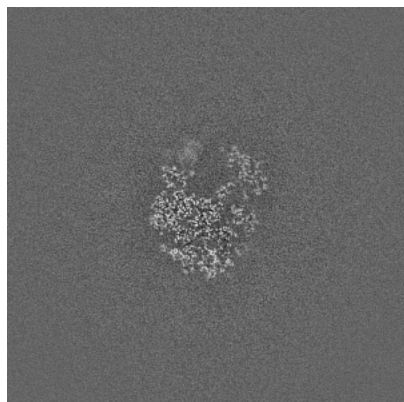


Z

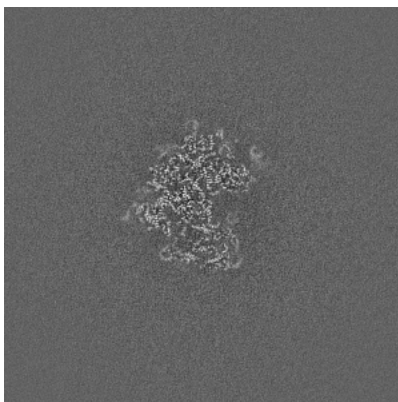
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

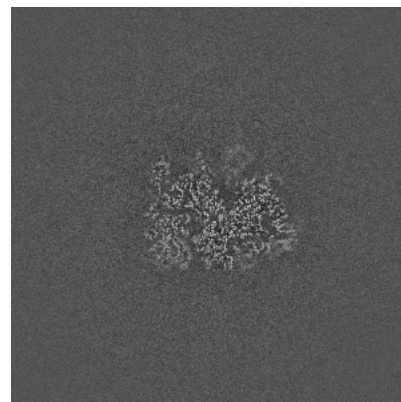
### 6.2.1 Primary map



X Index: 324

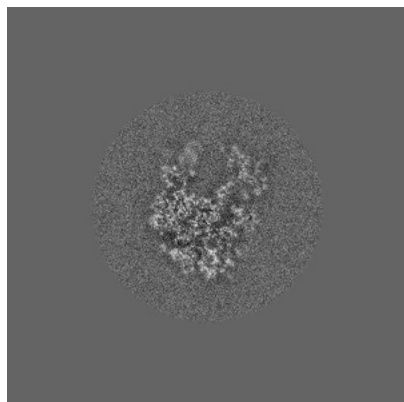


Y Index: 324

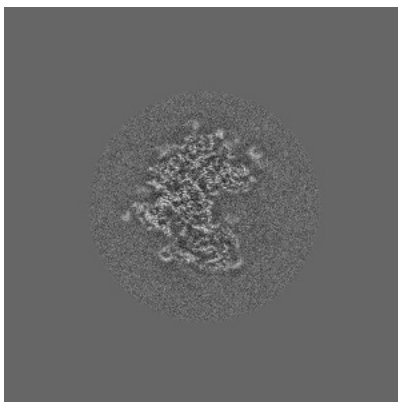


Z Index: 324

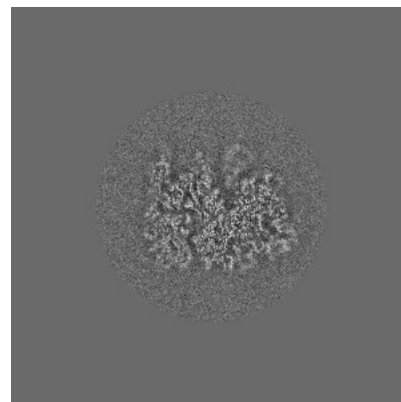
### 6.2.2 Raw map



X Index: 324



Y Index: 324

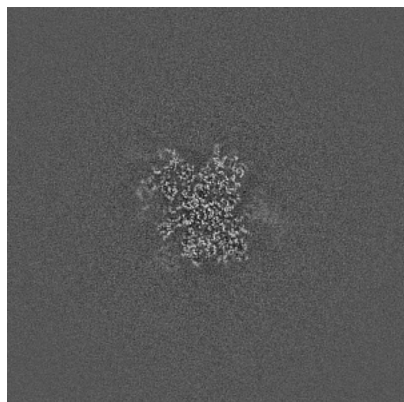


Z Index: 324

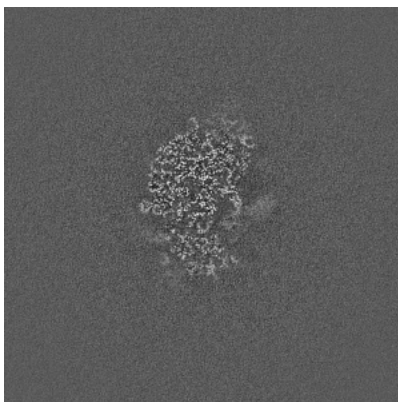
The images above show central slices of the map in three orthogonal directions.

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

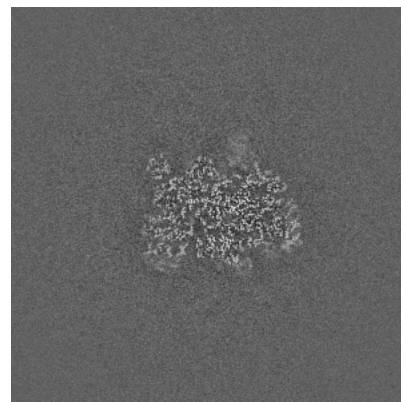
### 6.3.1 Primary map



X Index: 378

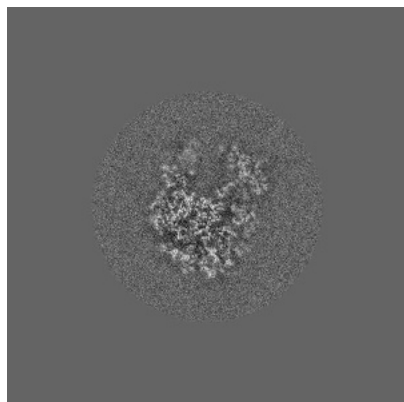


Y Index: 299

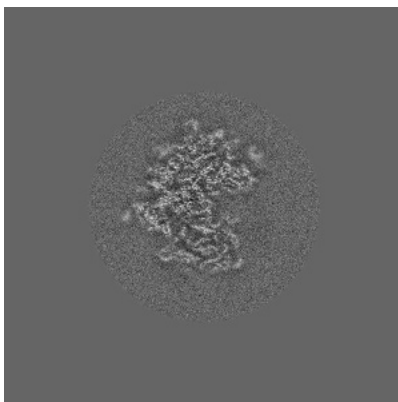


Z Index: 312

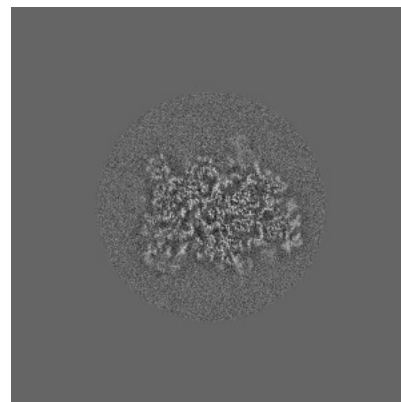
### 6.3.2 Raw map



X Index: 323



Y Index: 325



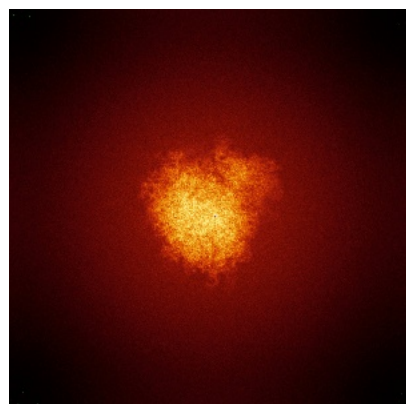
Z Index: 311

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

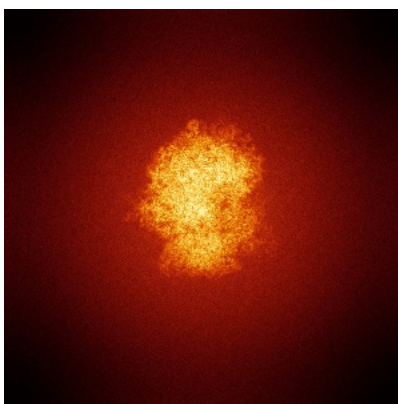


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

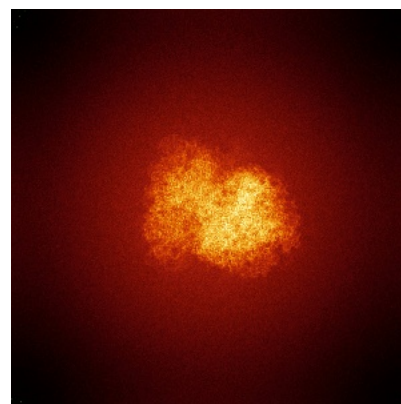
### 6.4.1 Primary map



X

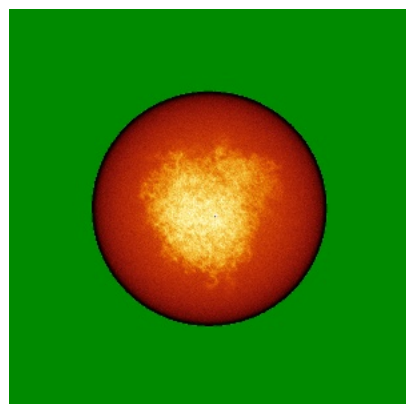


Y

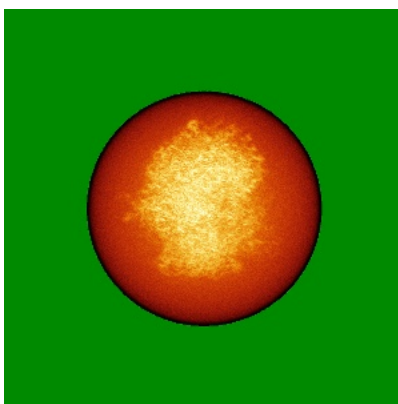


Z

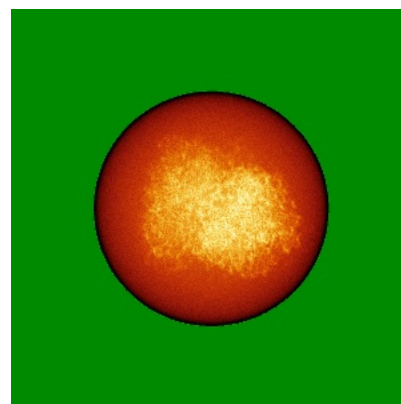
### 6.4.2 Raw map



X



Y

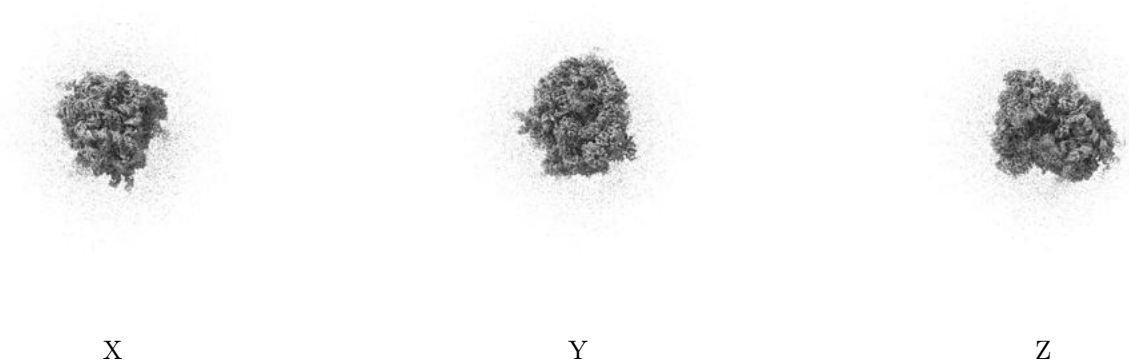


Z

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.

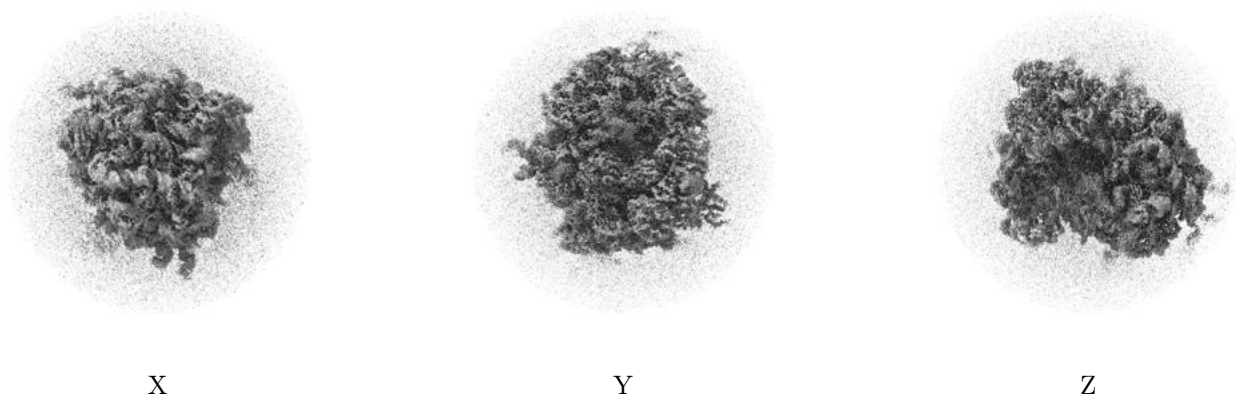
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 6.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

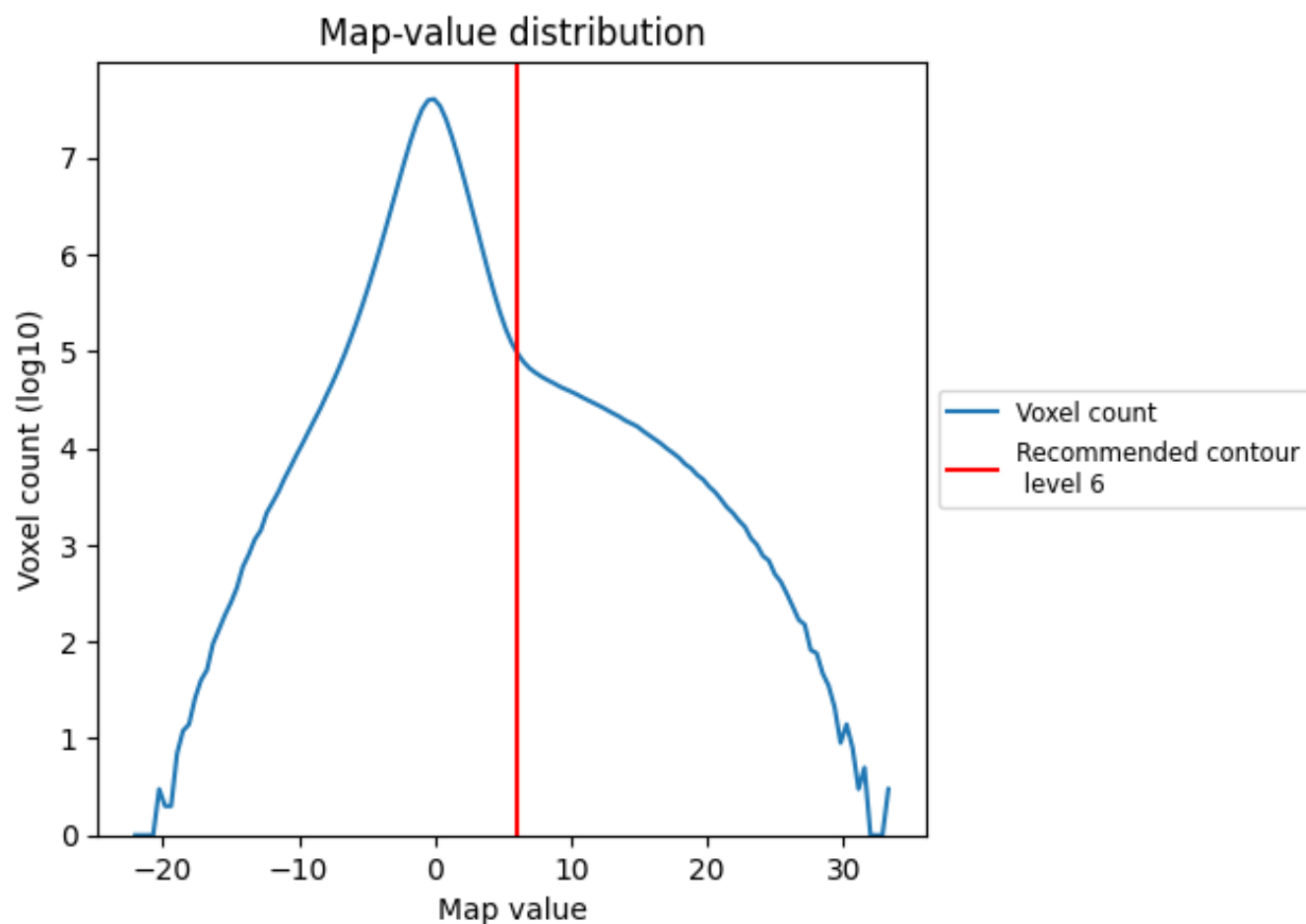
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

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

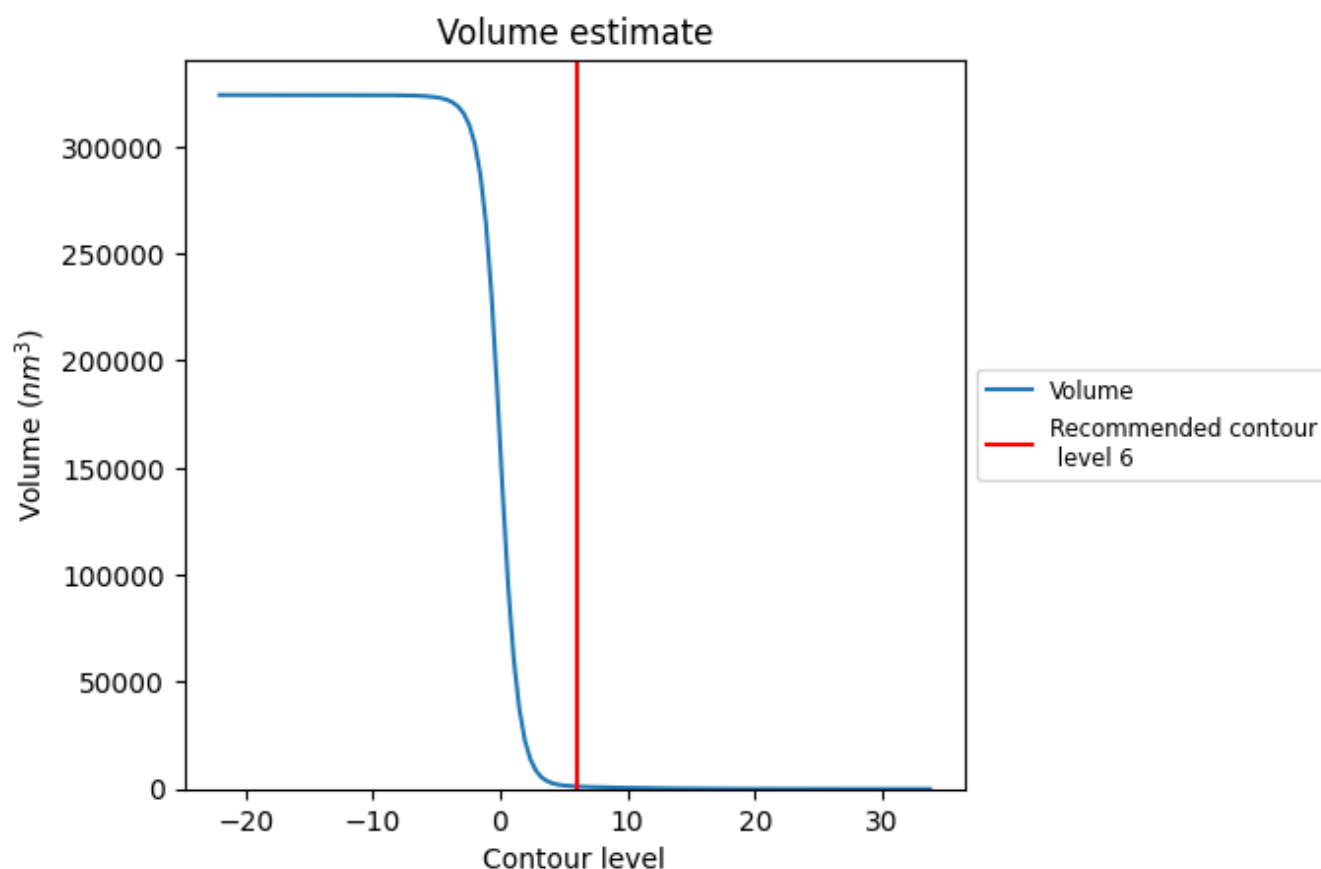
### 7.1 Map-value distribution [i](#)



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



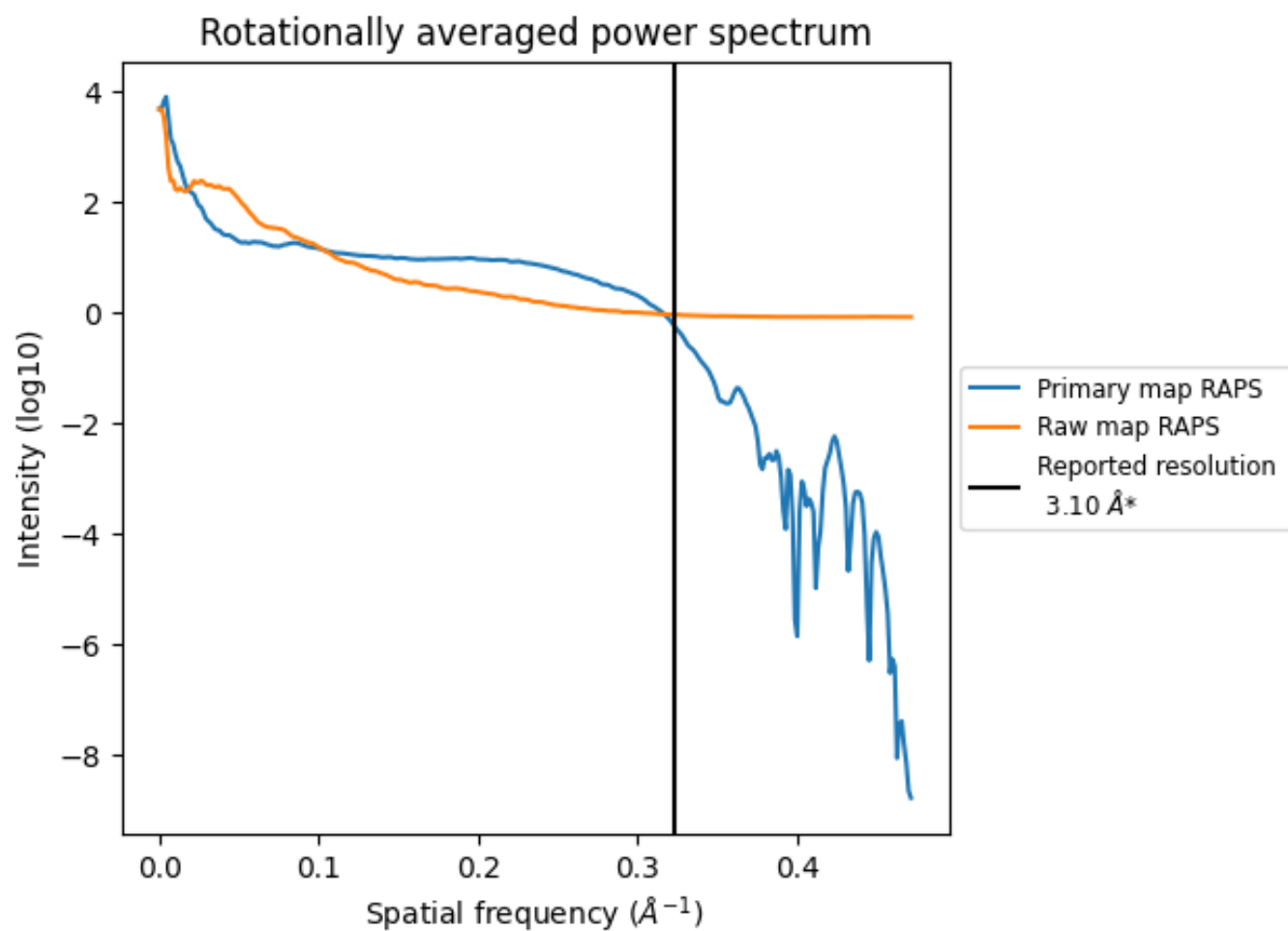
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1186  $\text{nm}^3$ ; this corresponds to an approximate mass of 1072 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 ⓘ

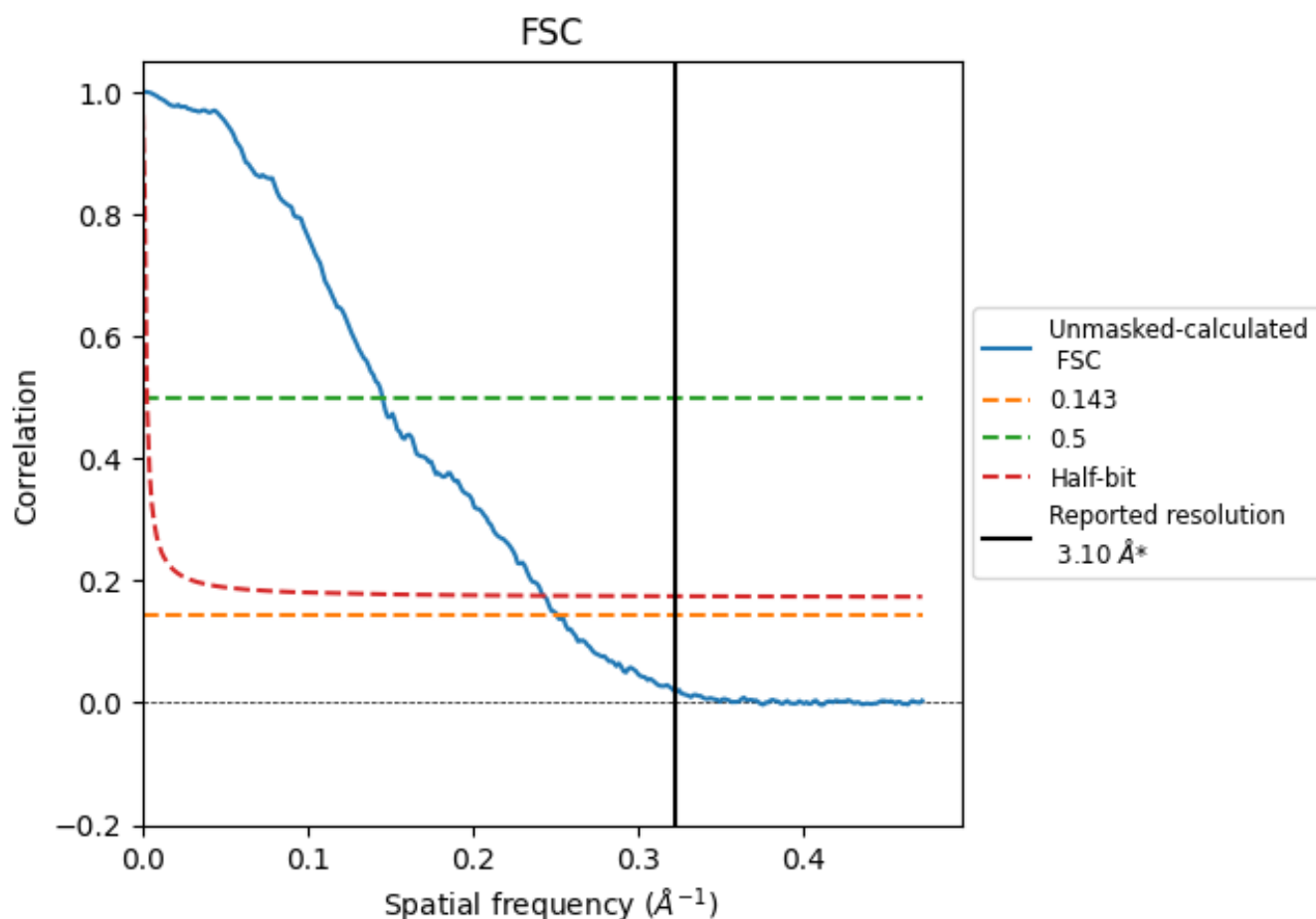


\*Reported resolution corresponds to spatial frequency of 0.323 Å<sup>-1</sup>

## 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 0.323  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

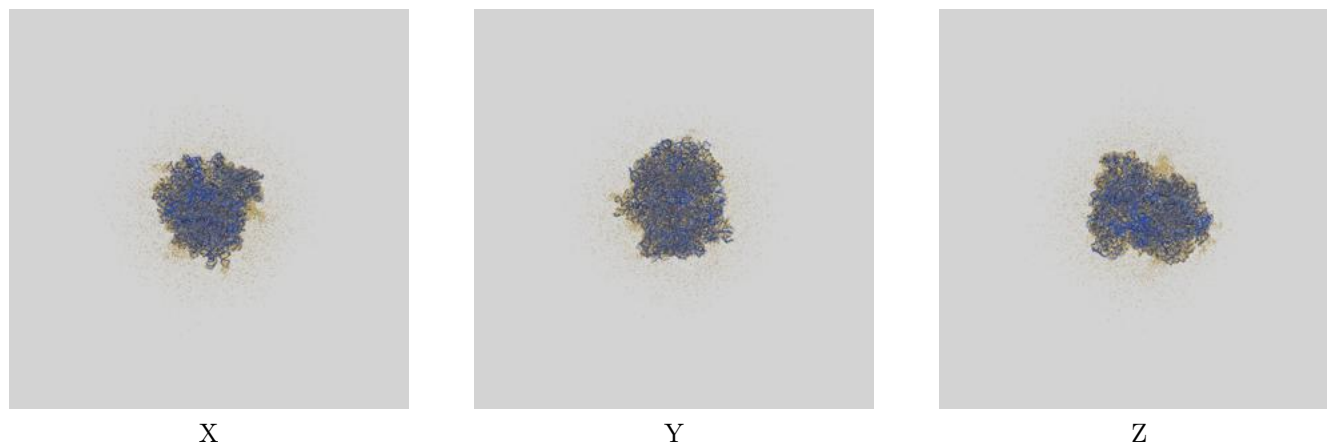
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 3.10                               | -    | -        |
| Author-provided FSC curve | -                                  | -    | -        |
| Unmasked-calculated*      | 3.99                               | 6.89 | 4.12     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.99 differs from the reported value 3.1 by more than 10 %

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

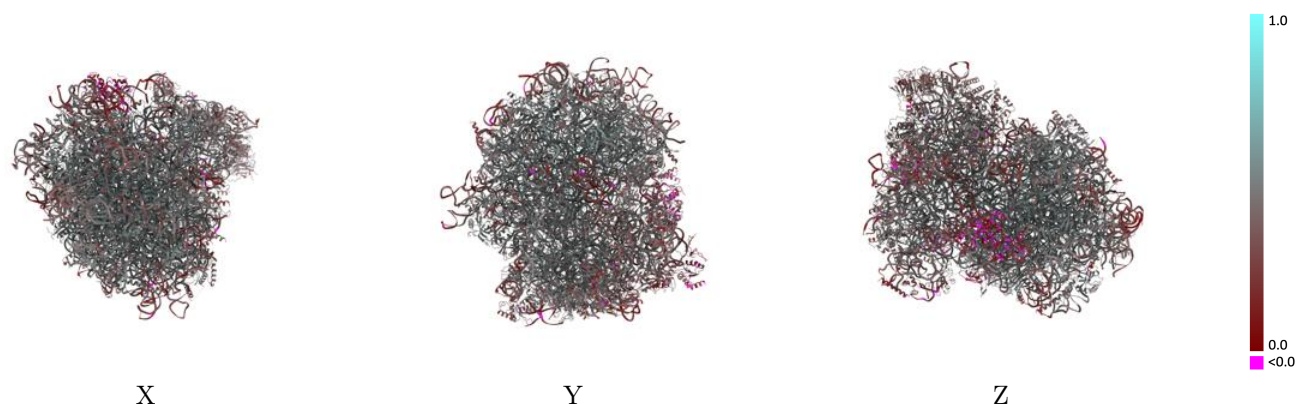
This section contains information regarding the fit between EMDB map EMD-43566 and PDB model 8VVR. Per-residue inclusion information can be found in [section 3](#) on [page 26](#).

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



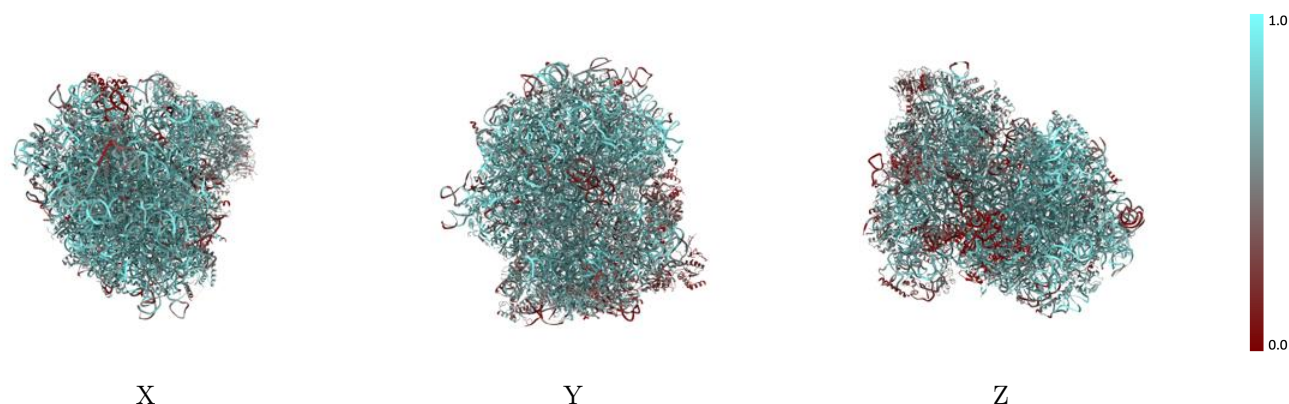
The images above show the 3D surface view of the map at the recommended contour level 6.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



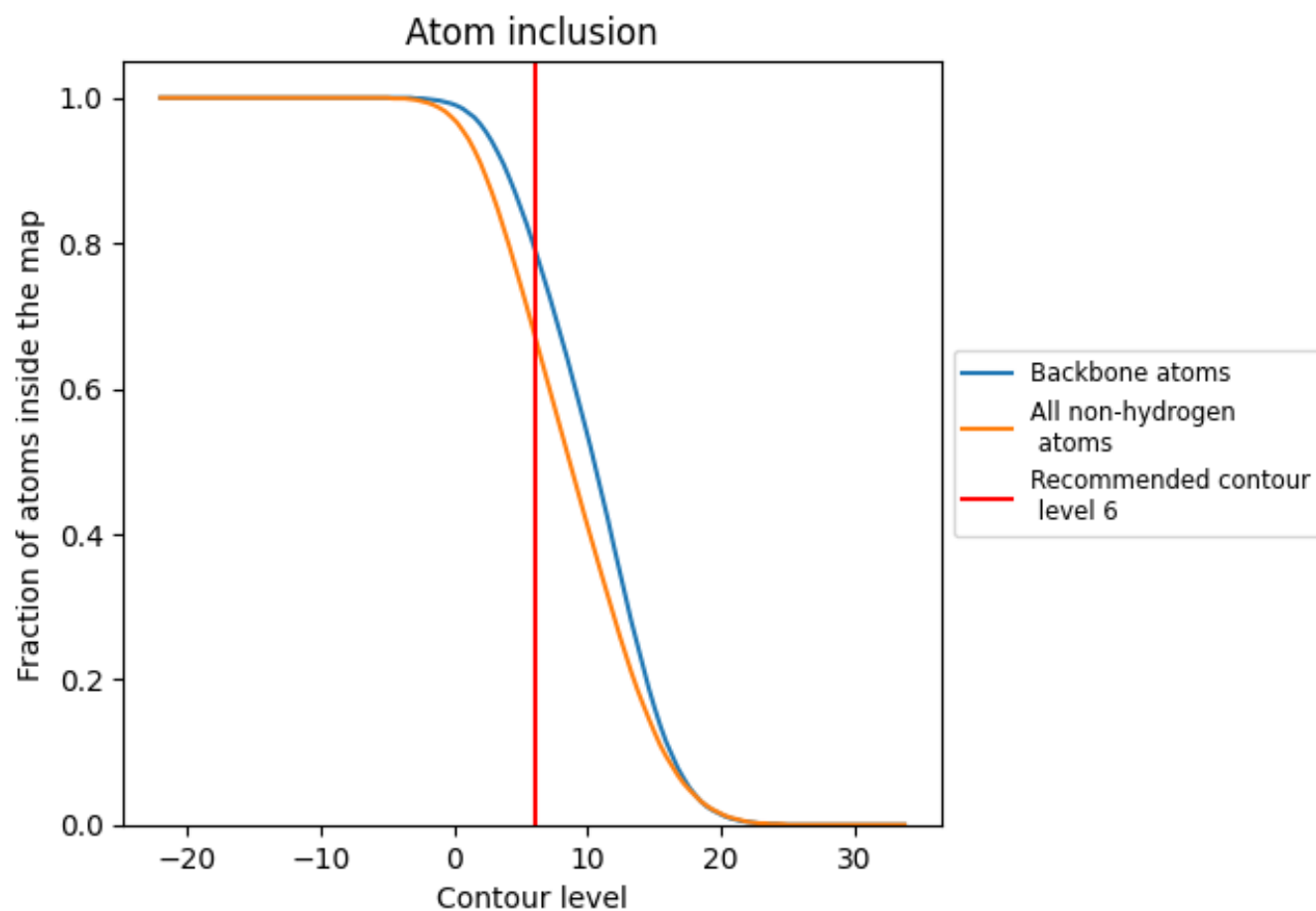
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (6).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 68% 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 (6) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.6750   |  0.4410   |
| A     |  0.7060   |  0.5200   |
| AA    |  0.5450   |  0.4210   |
| AB    |  0.5990   |  0.4410   |
| AC    |  0.6220   |  0.4750   |
| B     |  0.6880   |  0.4930   |
| BA    |  0.6640   |  0.4640   |
| BB    |  0.5780   |  0.4560   |
| BC    |  0.5540   |  0.4340   |
| C     |  0.6780   |  0.4980   |
| CA    |  0.6660   |  0.4830   |
| CB    |  0.6130   |  0.4630   |
| CC    |  0.5080   |  0.4150   |
| D     |  0.6790   |  0.4540   |
| DA    |  0.6810  |  0.5090  |
| DB    |  0.4850 |  0.3960 |
| DC    |  0.5910 |  0.4400 |
| E     |  0.6230 |  0.4470 |
| EA    |  0.6760 |  0.5190 |
| EB    |  0.5700 |  0.4510 |
| EC    |  0.4860 |  0.3880 |
| F     |  0.6670 |  0.4910 |
| FA    |  0.6590 |  0.4870 |
| FB    |  0.5380 |  0.4110 |
| FC    |  0.2160 |  0.2470 |
| G     |  0.6390 |  0.4380 |
| GA    |  0.6530 |  0.4700 |
| GB    |  0.4720 |  0.3630 |
| GC    |  0.3960 |  0.3440 |
| H     |  0.6500 |  0.4630 |
| HA    |  0.6510 |  0.4520 |
| HB    |  0.5010 |  0.3870 |
| HC    |  0.1340 |  0.2910 |
| I     |  0.6900 |  0.4970 |
| IA    |  0.7070 |  0.5150 |



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| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| IB    |  0.5690   |  0.4410   |
| IC    |  0.4500   |  0.4380   |
| J     |  0.6210   |  0.4360   |
| JA    |  0.5730   |  0.4280   |
| JB    |  0.5880   |  0.4320   |
| K     |  0.6560   |  0.4800   |
| KA    |  0.6350   |  0.4850   |
| KB    |  0.4820   |  0.3660   |
| L     |  0.6510   |  0.4610   |
| LA    |  0.7090   |  0.4940   |
| LB    |  0.6240   |  0.4810   |
| M     |  0.7110   |  0.5170   |
| MA    |  0.6470   |  0.4830   |
| MB    |  0.2220   |  0.2090   |
| N     |  0.6930   |  0.4880   |
| NA    |  0.6740   |  0.5080   |
| NB    |  0.6420   |  0.4630   |
| O     |  0.6750   |  0.4990   |
| OA    |  0.6700   |  0.5030   |
| OB    |  0.6030  |  0.4530  |
| P     |  0.6930 |  0.5050 |
| PA    |  0.6880 |  0.4970 |
| PB    |  0.4600 |  0.3640 |
| Q     |  0.6680 |  0.4640 |
| QB    |  0.5400 |  0.4130 |
| R     |  0.6790 |  0.4910 |
| RA    |  0.0400 |  0.0950 |
| RB    |  0.5420 |  0.4090 |
| S     |  0.6650 |  0.4890 |
| SA    |  0.6200 |  0.3980 |
| SB    |  0.5400 |  0.3980 |
| T     |  0.6020 |  0.4290 |
| TA    |  0.2320 |  0.2320 |
| TB    |  0.5440 |  0.4010 |
| U     |  0.6690 |  0.5050 |
| UA    |  0.2220 |  0.2550 |
| UB    |  0.4550 |  0.3760 |
| V     |  0.5090 |  0.3860 |
| VA    |  0.5440 |  0.4210 |
| VB    |  0.6220 |  0.4440 |
| W     |  0.6510 |  0.4700 |
| WA    |  0.7710 |  0.4530 |

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| Chain | Atom inclusion                                                                           | Q-score                                                                                  |
|-------|------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------|
| WB    |  0.6230 |  0.4740 |
| X     |  0.6600 |  0.4770 |
| XA    |  0.8620 |  0.4890 |
| XB    |  0.6020 |  0.4740 |
| Y     |  0.6940 |  0.4730 |
| YA    |  0.7790 |  0.4620 |
| YB    |  0.5050 |  0.3960 |
| Z     |  0.7280 |  0.5100 |
| ZA    |  0.7230 |  0.4300 |
| ZB    |  0.4480 |  0.3710 |
| b     |  0.0650 |  0.1310 |
| c     |  0.0180 |  0.1630 |