



## Full wwPDB EM Validation Report ⓘ

Jun 18, 2026 – 09:10 am BST

PDB ID : 6YDW / pdb\_00006ydw  
EMDB ID : EMD-10779  
Title : 55S mammalian mitochondrial ribosome with mtEFG1 and two tRNAMet (TI-POST)  
Authors : Kummer, E.; Ban, N.  
Deposited on : 2020-03-21  
Resolution : 4.20 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:

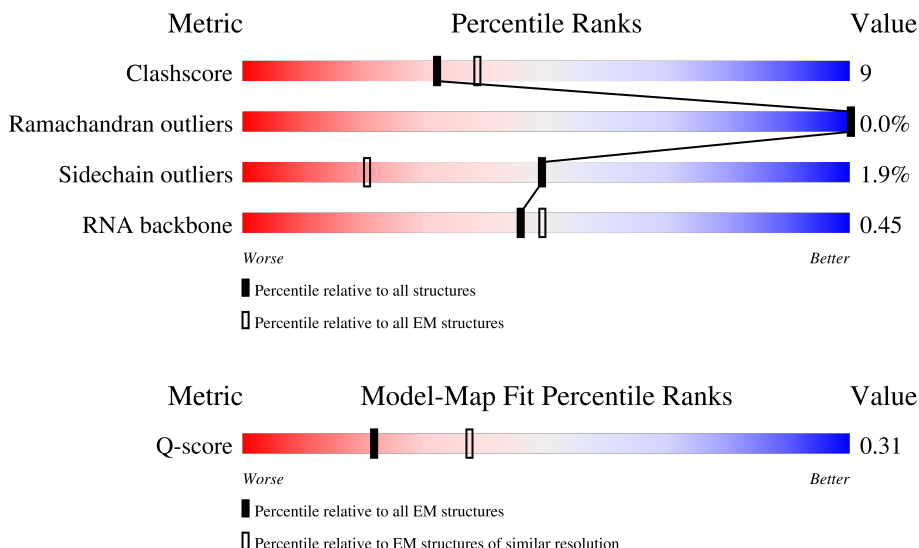
EMDB validation analysis : 0.0.1.dev132  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using 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 4.20 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                       | 5410 ( 3.70 - 4.70 )                                     |

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   | AI    | 397    | <div> <div>39%</div> <div>66%</div> <div>17%</div> <div>17%</div> </div> |
| 2   | BT    | 292    | <div> <div>61%</div> <div>15%</div> <div>24%</div> </div>                |
| 3   | BU    | 149    | <div> <div>6%</div> <div>75%</div> <div>19%</div> <div>6%</div> </div>   |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 4   | BV    | 209    |                  |
| 5   | BW    | 210    |                  |
| 6   | BX    | 150    |                  |
| 7   | BY    | 216    |                  |
| 8   | Ba    | 423    |                  |
| 9   | Bb    | 380    |                  |
| 10  | Bc    | 334    |                  |
| 11  | Bd    | 206    |                  |
| 12  | Be    | 135    |                  |
| 13  | Bf    | 142    |                  |
| 14  | Bg    | 159    |                  |
| 15  | Bh    | 332    |                  |
| 16  | Bi    | 306    |                  |
| 17  | Bj    | 279    |                  |
| 18  | Bk    | 269    |                  |
| 19  | Bl    | 166    |                  |
| 20  | Bm    | 198    |                  |
| 21  | Bn    | 128    |                  |
| 22  | Bo    | 124    |                  |
| 23  | Bp    | 112    |                  |
| 24  | Bq    | 138    |                  |
| 25  | Bt    | 102    |                  |
| 26  | Bu    | 205    |                  |
| 27  | Bv    | 222    |                  |
| 28  | B0    | 148    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 29  | Bw    | 433    |                  |
| 30  | Bx    | 196    |                  |
| 31  | AA    | 16770  |                  |
| 31  | BA    | 16770  |                  |
| 32  | AB    | 289    |                  |
| 33  | AC    | 167    |                  |
| 34  | AE    | 430    |                  |
| 35  | AF    | 276    |                  |
| 36  | AG    | 242    |                  |
| 37  | AJ    | 200    |                  |
| 38  | AK    | 196    |                  |
| 39  | AL    | 139    |                  |
| 40  | AN    | 128    |                  |
| 41  | AO    | 239    |                  |
| 42  | AP    | 135    |                  |
| 43  | AQ    | 130    |                  |
| 44  | AR    | 143    |                  |
| 45  | AU    | 87     |                  |
| 46  | AV    | 71     |                  |
| 46  | AY    | 71     |                  |
| 47  | AX    | 6      |                  |
| 48  | AZ    | 18     |                  |
| 49  | Aa    | 382    |                  |
| 50  | Ab    | 190    |                  |
| 51  | Ac    | 173    |                  |

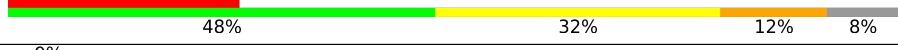
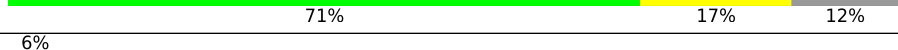
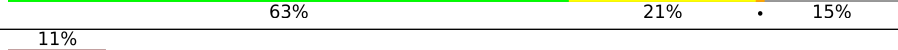
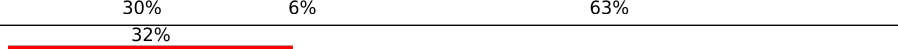
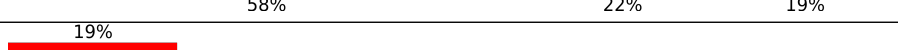
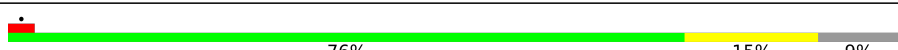
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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 52  | Ad    | 205    |                  |
| 53  | Ae    | 455    |                  |
| 54  | B1    | 256    |                  |
| 55  | Af    | 188    |                  |
| 56  | Ag    | 410    |                  |
| 57  | Ah    | 387    |                  |
| 58  | Ai    | 106    |                  |
| 59  | Aj    | 218    |                  |
| 60  | Ak    | 325    |                  |
| 61  | Am    | 118    |                  |
| 62  | An    | 199    |                  |
| 63  | Ao    | 692    |                  |
| 64  | Ap    | 258    |                  |
| 65  | CL    | 198    |                  |
| 65  | DL    | 198    |                  |
| 65  | EL    | 198    |                  |
| 65  | FL    | 198    |                  |
| 65  | GL    | 198    |                  |
| 65  | HL    | 198    |                  |
| 65  | LL    | 198    |                  |
| 66  | B2    | 252    |                  |
| 67  | B3    | 161    |                  |
| 68  | B4    | 126    |                  |
| 69  | B5    | 188    |                  |
| 70  | B6    | 65     |                  |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 71  | B7    | 95     |    |
| 72  | B8    | 188    |    |
| 73  | B9    | 100    |    |
| 74  | BB    | 73     |    |
| 75  | BC    | 721    |    |
| 76  | BD    | 306    |    |
| 77  | BE    | 348    |    |
| 78  | BF    | 294    |    |
| 79  | BI    | 268    |    |
| 80  | BJ    | 262    |    |
| 81  | BK    | 192    |    |
| 82  | BN    | 178    |  |
| 83  | BO    | 145    |  |
| 84  | BP    | 296    |  |
| 85  | BQ    | 251    |  |
| 86  | BR    | 169    |  |
| 87  | BS    | 180    |  |

## 2 Entry composition

There are 95 unique types of molecules in this entry. The entry contains 180836 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 Uncharacterized protein.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1   | AI    | 328      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2650  | 1678 | 478 | 481 | 13 |         |       |

- Molecule 2 is a protein called Mitochondrial ribosomal protein L19.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 2   | BT    | 222      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1840  | 1178 | 318 | 335 | 9 |         |       |

- Molecule 3 is a protein called Mitochondrial ribosomal protein L20.

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

- Molecule 4 is a protein called Mitochondrial ribosomal protein L21.

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

- Molecule 5 is a protein called Uncharacterized protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 5   | BW    | 166      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1374  | 876 | 258 | 234 | 6 |         |       |

- Molecule 6 is a protein called Uncharacterized protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 6   | BX    | 149      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1181  | 752 | 227 | 200 | 2 |         |       |

- Molecule 7 is a protein called Uncharacterized protein.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 7   | BY    | 206      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1678  | 1056 | 308 | 309 | 5 |         |       |

- Molecule 8 is a protein called Mitochondrial ribosomal protein L37.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 8   | Ba    | 393      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3173  | 2040 | 556 | 565 | 12 |         |       |

- Molecule 9 is a protein called Mitochondrial ribosomal protein L38.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 9   | Bb    | 354      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2952  | 1876 | 542 | 525 | 9 |         |       |

- Molecule 10 is a protein called Mitochondrial ribosomal protein L39.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 10  | Bc    | 295      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2408  | 1541 | 410 | 441 | 16 |         |       |

- Molecule 11 is a protein called Uncharacterized protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 11  | Bd    | 140      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1177  | 742 | 213 | 221 | 1 |         |       |

- Molecule 12 is a protein called Mitochondrial ribosomal protein L41.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 12  | Be    | 122      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 972   | 628 | 168 | 173 | 3 |         |       |

- Molecule 13 is a protein called Uncharacterized protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 13  | Bf    | 108      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 827   | 519 | 154 | 150 | 4 |         |       |

- Molecule 14 is a protein called Mitochondrial ribosomal protein L43.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 14  | Bg    | 148      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1167  | 727 | 225 | 212 | 3 |         |       |

- Molecule 15 is a protein called Uncharacterized protein.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 15  | Bh    | 289      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2319  | 1486 | 399 | 426 | 8 |         |       |

- Molecule 16 is a protein called Mitochondrial ribosomal protein L45.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 16  | Bi    | 260      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2138  | 1370 | 379 | 379 | 10 |         |       |

- Molecule 17 is a protein called Mitochondrial ribosomal protein L46.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 17  | Bj    | 217      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1775  | 1137 | 311 | 321 | 6 |         |       |

- Molecule 18 is a protein called 39S ribosomal protein L48, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 18  | Bk    | 155      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1246  | 796 | 214 | 231 | 5 |         |       |

- Molecule 19 is a protein called Mrpl34.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19  | Bl    | 133      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1097  | 709 | 192 | 194 | 2 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference      |
|-------|---------|----------|--------|----------|----------------|
| Bl    | 59      | ARG      | LYS    | conflict | UNP A0A0R4J8D6 |

- Molecule 20 is a protein called Mitochondrial ribosomal protein L50.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 20  | Bm    | 109      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 893   | 568 | 160 | 162 | 3 |         |       |

- Molecule 21 is a protein called Mitochondrial ribosomal protein L51.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 21  | Bn    | 97       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 837   | 539 | 166 | 128 | 4 |         |       |

- Molecule 22 is a protein called Uncharacterized protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 22  | Bo    | 97       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 772   | 481 | 148 | 141 | 2 |         |       |

- Molecule 23 is a protein called mL53.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 23  | Bp    | 97       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 742   | 459 | 143 | 134 | 6 |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference      |
|-------|---------|----------|--------|----------|----------------|
| Bp    | 12      | ALA      | SER    | conflict | UNP A0A341D604 |
| Bp    | 107     | SER      | GLY    | conflict | UNP A0A341D604 |

- Molecule 24 is a protein called Uncharacterized protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 24  | Bq    | 85       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 697   | 446 | 128 | 121 | 2 |         |       |

- Molecule 25 is a protein called Mitochondrial ribosomal protein L57.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 25  | Bt    | 94       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 780   | 485 | 168 | 126 | 1 |         |       |

- Molecule 26 is a protein called Uncharacterized protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 26  | Bu    | 151      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1198  | 738 | 233 | 222 | 5 |         |       |

- Molecule 27 is a protein called Uncharacterized protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 27  | Bv    | 135      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1131  | 692 | 223 | 211 | 5 |         |       |

- Molecule 28 is a protein called Mitochondrial ribosomal protein L27.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 28  | B0    | 110      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 857   | 553 | 156 | 145 | 3 |         |       |

- Molecule 29 is a protein called 39S ribosomal protein S30, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 29  | Bw    | 387      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3126  | 2011 | 548 | 555 | 12 |         |       |

- Molecule 30 is a protein called Mitochondrial ribosomal protein S18A.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 30  | Bx    | 162      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1325  | 845 | 249 | 224 | 7 |         |       |

- Molecule 31 is a RNA chain called 12S rRNA.

| Mol | Chain | Residues | Atoms |       |      |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|-------|
| 31  | AA    | 960      | Total | C     | N    | O     | P    | 0       | 0     |
|     |       |          | 20411 | 9162  | 3708 | 6581  | 960  |         |       |
| 31  | BA    | 1544     | Total | C     | N    | O     | P    | 0       | 0     |
|     |       |          | 32844 | 14750 | 5972 | 10578 | 1544 |         |       |

There are 20 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference    |
|-------|---------|----------|--------|----------|--------------|
| AA    | 2316    | G        | A      | conflict | GB 347448639 |
| AA    | 2973    | C        | U      | conflict | GB 347448639 |
| AA    | 11929   | C        | U      | conflict | GB 347448639 |
| AA    | 12670   | C        | U      | conflict | GB 347448639 |

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| Chain | Residue | Modelled | Actual | Comment  | Reference    |
|-------|---------|----------|--------|----------|--------------|
| AA    | 13439   | A        | G      | conflict | GB 347448639 |
| AA    | 14686   | A        | C      | conflict | GB 347448639 |
| AA    | 15015   | G        | A      | conflict | GB 347448639 |
| AA    | 15689   | U        | C      | conflict | GB 347448639 |
| AA    | 15828   | G        | C      | conflict | GB 347448639 |
| AA    | 16058   | G        | A      | conflict | GB 347448639 |
| BA    | 1287    | G        | A      | conflict | GB 347448639 |
| BA    | 1944    | C        | U      | conflict | GB 347448639 |
| BA    | 10900   | C        | U      | conflict | GB 347448639 |
| BA    | 11641   | C        | U      | conflict | GB 347448639 |
| BA    | 12410   | A        | G      | conflict | GB 347448639 |
| BA    | 13657   | A        | C      | conflict | GB 347448639 |
| BA    | 13986   | G        | A      | conflict | GB 347448639 |
| BA    | 14660   | U        | C      | conflict | GB 347448639 |
| BA    | 14799   | G        | C      | conflict | GB 347448639 |
| BA    | 15029   | G        | A      | conflict | GB 347448639 |

- Molecule 32 is a protein called Mitochondrial ribosomal protein S2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 32  | AB    | 220      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1762  | 1126 | 326 | 304 | 6 |         |       |

- Molecule 33 is a protein called Mitochondrial ribosomal protein S24.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 33  | AC    | 132      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1075  | 695 | 195 | 181 | 4 |         |       |

- Molecule 34 is a protein called Mitochondrial ribosomal protein S5.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 34  | AE    | 343      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2732  | 1707 | 527 | 487 | 11 |         |       |

- Molecule 35 is a protein called Uncharacterized protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 35  | AF    | 122      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 981   | 620 | 178 | 177 | 6 |         |       |

- Molecule 36 is a protein called Mitochondrial ribosomal protein S7.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 36  | AG    | 208      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1721  | 1097 | 314 | 299 | 11 |         |       |

- Molecule 37 is a protein called Mitochondrial ribosomal protein S10.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 37  | AJ    | 140      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1155  | 746 | 197 | 208 | 4 |         |       |

- Molecule 38 is a protein called uS11m.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 38  | AK    | 137      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1007  | 631 | 193 | 180 | 3 |         |       |

- Molecule 39 is a protein called Mitochondrial ribosomal protein S12.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 39  | AL    | 109      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 840   | 524 | 172 | 138 | 6 |         |       |

- Molecule 40 is a protein called Mitochondrial ribosomal protein S14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 40  | AN    | 101      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 858   | 534 | 174 | 144 | 6 |         |       |

- Molecule 41 is a protein called uS15m.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 41  | AO    | 175      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1448  | 919 | 272 | 248 | 9 |         |       |

- Molecule 42 is a protein called 28S ribosomal protein S16, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 42  | AP    | 117      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 932   | 588 | 184 | 155 | 5 |         |       |

- Molecule 43 is a protein called uS17m.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 43  | AQ    | 112      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 875   | 568 | 153 | 151 | 3 |         |       |

- Molecule 44 is a protein called Mitochondrial ribosomal protein S18C.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 44  | AR    | 97       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 784   | 507 | 132 | 138 | 7 |         |       |

- Molecule 45 is a protein called bS21m.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 45  | AU    | 86       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 734   | 453 | 148 | 125 | 8 |         |       |

- Molecule 46 is a RNA chain called tRNAMet.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 46  | AV    | 71       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1498  | 673 | 264 | 491 | 70 |         |       |
| 46  | AY    | 71       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1498  | 673 | 264 | 491 | 70 |         |       |

There are 6 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment   | Reference     |
|-------|---------|----------|--------|-----------|---------------|
| AV    | 69      | C        | -      | insertion | GB 1208989970 |
| AV    | 70      | C        | -      | insertion | GB 1208989970 |
| AV    | 71      | A        | -      | insertion | GB 1208989970 |
| AY    | 69      | C        | -      | insertion | GB 1208989970 |
| AY    | 70      | C        | -      | insertion | GB 1208989970 |
| AY    | 71      | A        | -      | insertion | GB 1208989970 |

- Molecule 47 is a RNA chain called mRNA.

| Mol | Chain | Residues | Atoms |    |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|-------|
| 47  | AX    | 6        | Total | C  | N  | O  | P | 0       | 0     |
|     |       |          | 128   | 57 | 22 | 43 | 6 |         |       |

- Molecule 48 is a protein called unknown peptide.

| Mol | Chain | Residues | Atoms |    |    |    | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|-------|
| 48  | AZ    | 18       | Total | C  | N  | O  | 0       | 0     |
|     |       |          | 90    | 54 | 18 | 18 |         |       |

- Molecule 49 is a protein called Mitochondrial ribosomal protein S22.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 49  | Aa    | 292      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2378  | 1518 | 409 | 442 | 9 |         |       |

- Molecule 50 is a protein called mS23.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 50  | Ab    | 135      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1101  | 709 | 199 | 192 | 1 |         |       |

- Molecule 51 is a protein called Mitochondrial ribosomal protein S25.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 51  | Ac    | 169      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1367  | 876 | 236 | 245 | 10 |         |       |

- Molecule 52 is a protein called Mitochondrial ribosomal protein S26.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 52  | Ad    | 177      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1467  | 904 | 288 | 273 | 2 |         |       |

- Molecule 53 is a protein called Mitochondrial ribosomal protein S27.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 53  | Ae    | 388      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3109  | 1971 | 535 | 589 | 14 |         |       |

- Molecule 54 is a protein called Mitochondrial ribosomal protein L28.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 54  | B1    | 244      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2036  | 1315 | 363 | 353 | 5 |         |       |

- Molecule 55 is a protein called Mitoribosomal protein ms28, mrps28.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 55  | Af    | 99       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 778   | 494 | 134 | 146 | 4 |         |       |

- Molecule 56 is a protein called Death associated protein 3.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 56  | Ag    | 353      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2875  | 1837 | 515 | 513 | 10 |         |       |

- Molecule 57 is a protein called Mitochondrial ribosomal protein S31.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 57  | Ah    | 120      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1015  | 659 | 168 | 185 | 3 |         |       |

There are 10 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment   | Reference  |
|-------|---------|----------|--------|-----------|------------|
| Ah    | 180     | UNK      | -      | insertion | UNP F1RME2 |
| Ah    | 181     | GLN      | -      | insertion | UNP F1RME2 |
| Ah    | 182     | LYS      | -      | insertion | UNP F1RME2 |
| Ah    | 184     | GLY      | -      | insertion | UNP F1RME2 |
| Ah    | 185     | GLU      | LYS    | conflict  | UNP F1RME2 |
| Ah    | 187     | PRO      | LYS    | conflict  | UNP F1RME2 |
| Ah    | 189     | ILE      | LEU    | conflict  | UNP F1RME2 |
| Ah    | 190     | SER      | ILE    | conflict  | UNP F1RME2 |
| Ah    | 237     | SER      | -      | insertion | UNP F1RME2 |
| Ah    | 238     | PHE      | -      | insertion | UNP F1RME2 |

- Molecule 58 is a protein called mS33.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 58  | Ai    | 99       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 824   | 522 | 156 | 143 | 3 |         |       |

- Molecule 59 is a protein called mS34.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 59  | Aj    | 213      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1788  | 1131 | 338 | 311 | 8 |         |       |

- Molecule 60 is a protein called Mitochondrial ribosomal protein S35.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 60  | Ak    | 275      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2222  | 1414 | 380 | 419 | 9 |         |       |

- Molecule 61 is a protein called mS37.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 61  | Am    | 116      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 930   | 577 | 185 | 160 | 8 |         |       |

- Molecule 62 is a protein called Aurora kinase A interacting protein 1.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 62  | An    | 72       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 639   | 407 | 139 | 92 | 1 |         |       |

- Molecule 63 is a protein called mS39.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 63  | Ao    | 572      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 4525  | 2897 | 770 | 834 | 24 |         |       |

- Molecule 64 is a protein called 28S ribosomal protein S18b, mitochondrial.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 64  | Ap    | 190      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1564  | 991 | 292 | 273 | 8 |         |       |

- Molecule 65 is a protein called Mitochondrial ribosomal protein L12.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 65  | CL    | 45       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 317   | 203 | 52 | 62 |         |       |
| 65  | DL    | 27       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 213   | 137 | 33 | 43 |         |       |
| 65  | EL    | 28       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 222   | 143 | 35 | 44 |         |       |
| 65  | FL    | 27       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 213   | 137 | 33 | 43 |         |       |
| 65  | GL    | 27       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 213   | 137 | 33 | 43 |         |       |
| 65  | HL    | 26       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 205   | 131 | 32 | 42 |         |       |

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| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 65  | LL    | 70       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 537   | 346 | 93 | 98 |         |       |

- Molecule 66 is a protein called Mitochondrial ribosomal protein L47.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 66  | B2    | 179      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1548  | 992 | 290 | 260 | 6 |         |       |

- Molecule 67 is a protein called Uncharacterized protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 67  | B3    | 118      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 968   | 622 | 178 | 165 | 3 |         |       |

- Molecule 68 is a protein called Uncharacterized protein.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 68  | B4    | 62       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 474   | 296 | 94 | 81 | 3 |         |       |

- Molecule 69 is a protein called Uncharacterized protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 69  | B5    | 110      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 902   | 553 | 181 | 162 | 6 |         |       |

- Molecule 70 is a protein called Uncharacterized protein.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 70  | B6    | 52       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 425   | 274 | 78 | 71 | 2 |         |       |

- Molecule 71 is a protein called Mitochondrial ribosomal protein L34.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 71  | B7    | 46       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 387   | 239 | 89 | 58 | 1 |         |       |

- Molecule 72 is a protein called Mitochondrial ribosomal protein L35.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 72  | B8    | 95       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 833   | 539 | 163 | 129 | 2 |         |       |

- Molecule 73 is a protein called Ribosomal protein.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 73  | B9    | 38       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 335   | 214 | 70 | 47 | 4 |         |       |

- Molecule 74 is a RNA chain called CP tRNA-Phe.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 74  | BB    | 67       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1427  | 640 | 261 | 459 | 67 |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment   | Reference   |
|-------|---------|----------|--------|-----------|-------------|
| BB    | 72      | C        | -      | insertion | GB 76262549 |
| BB    | 73      | A        | -      | insertion | GB 76262549 |

- Molecule 75 is a protein called Elongation factor G, mitochondrial.

| Mol | Chain | Residues | Atoms |      |     |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|----|---------|-------|
| 75  | BC    | 694      | Total | C    | N   | O    | S  | 0       | 0     |
|     |       |          | 5425  | 3422 | 935 | 1035 | 33 |         |       |

There are 6 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| BC    | 31      | GLY      | -      | expression tag | UNP Q96RP9 |
| BC    | 32      | GLY      | -      | expression tag | UNP Q96RP9 |
| BC    | 33      | SER      | -      | expression tag | UNP Q96RP9 |
| BC    | 34      | GLY      | -      | expression tag | UNP Q96RP9 |
| BC    | 35      | SER      | -      | expression tag | UNP Q96RP9 |
| BC    | 36      | GLY      | -      | expression tag | UNP Q96RP9 |

- Molecule 76 is a protein called Uncharacterized protein.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 76  | BD    | 240      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1860  | 1160 | 371 | 319 | 10 |         |       |

- Molecule 77 is a protein called ICT1.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 77  | BE    | 307      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2420  | 1554 | 426 | 430 | 10 |         |       |

- Molecule 78 is a protein called Mitochondrial ribosomal protein L4.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 78  | BF    | 250      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2011  | 1294 | 367 | 344 | 6 |         |       |

- Molecule 79 is a protein called Mitochondrial ribosomal protein L9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 79  | BI    | 98       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 805   | 509 | 155 | 141 |   |         |       |

- Molecule 80 is a protein called Mitochondrial ribosomal protein L10.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 80  | BJ    | 212      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1705  | 1100 | 306 | 290 | 9 |         |       |

- Molecule 81 is a protein called Mitochondrial ribosomal protein L11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 81  | BK    | 176      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1339  | 851 | 243 | 243 | 2 |         |       |

- Molecule 82 is a protein called Uncharacterized protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 82  | BN    | 177      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1444  | 926 | 258 | 253 | 7 |         |       |

- Molecule 83 is a protein called Uncharacterized protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 83  | BO    | 115      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 896   | 562 | 176 | 154 | 4 |         |       |

- Molecule 84 is a protein called Uncharacterized protein.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 84  | BP    | 288      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2312  | 1473 | 430 | 403 | 6 |         |       |

- Molecule 85 is a protein called Uncharacterized protein.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 85  | BQ    | 222      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1803  | 1156 | 331 | 306 | 10 |         |       |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| BQ    | 237     | HIS      | TYR    | conflict | UNP F1RI89 |

- Molecule 86 is a protein called Uncharacterized protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 86  | BR    | 153      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1240  | 777 | 236 | 222 | 5 |         |       |

- Molecule 87 is a protein called Mitochondrial ribosomal protein L18.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 87  | BS    | 143      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1168  | 733 | 227 | 204 | 4 |         |       |

- Molecule 88 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |     | AltConf |
|-----|-------|----------|-------|-----|---------|
| 88  | BW    | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 88  | Be    | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 88  | Bl    | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 88  | Bq    | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 88  | Bt    | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 88  | B0    | 1        | Total | Mg  | 0       |
|     |       |          | 1     | 1   |         |
| 88  | AA    | 102      | Total | Mg  | 0       |
|     |       |          | 102   | 102 |         |

*Continued on next page...*

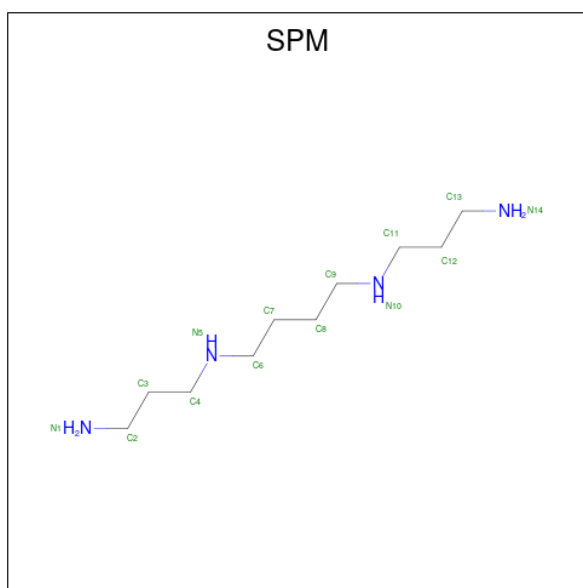
*Continued from previous page...*

| Mol | Chain | Residues | Atoms        |           | AltConf |
|-----|-------|----------|--------------|-----------|---------|
| 88  | AB    | 1        | Total<br>1   | Mg<br>1   | 0       |
| 88  | AX    | 1        | Total<br>1   | Mg<br>1   | 0       |
| 88  | Ag    | 1        | Total<br>1   | Mg<br>1   | 0       |
| 88  | Am    | 1        | Total<br>1   | Mg<br>1   | 0       |
| 88  | An    | 1        | Total<br>1   | Mg<br>1   | 0       |
| 88  | BA    | 200      | Total<br>200 | Mg<br>200 | 0       |
| 88  | BB    | 1        | Total<br>1   | Mg<br>1   | 0       |
| 88  | BC    | 2        | Total<br>2   | Mg<br>2   | 0       |
| 88  | BD    | 3        | Total<br>3   | Mg<br>3   | 0       |
| 88  | BF    | 1        | Total<br>1   | Mg<br>1   | 0       |
| 88  | BJ    | 1        | Total<br>1   | Mg<br>1   | 0       |
| 88  | BP    | 3        | Total<br>3   | Mg<br>3   | 0       |
| 88  | BQ    | 1        | Total<br>1   | Mg<br>1   | 0       |

- Molecule 89 is ZINC ION (CCD ID: ZN) (formula: Zn).

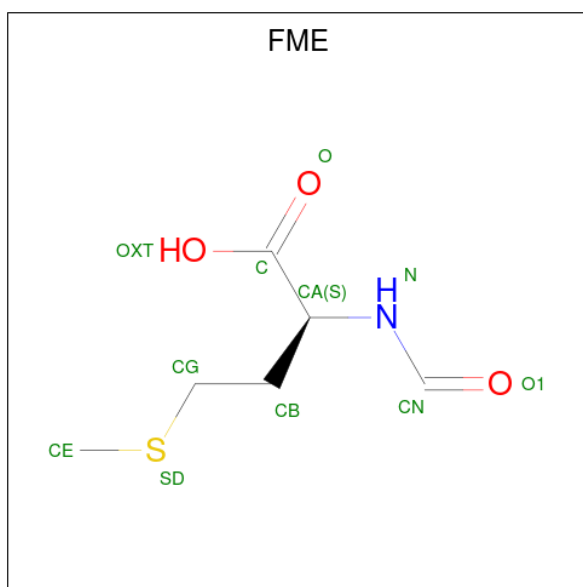
| Mol | Chain | Residues | Atoms      |         | AltConf |
|-----|-------|----------|------------|---------|---------|
| 89  | Bx    | 1        | Total<br>1 | Zn<br>1 | 0       |
| 89  | AR    | 1        | Total<br>1 | Zn<br>1 | 0       |
| 89  | Ac    | 1        | Total<br>1 | Zn<br>1 | 0       |
| 89  | Ap    | 1        | Total<br>1 | Zn<br>1 | 0       |
| 89  | B5    | 1        | Total<br>1 | Zn<br>1 | 0       |
| 89  | B9    | 1        | Total<br>1 | Zn<br>1 | 0       |

- Molecule 90 is SPERMINE (CCD ID: SPM) (formula:  $C_{10}H_{26}N_4$ ).



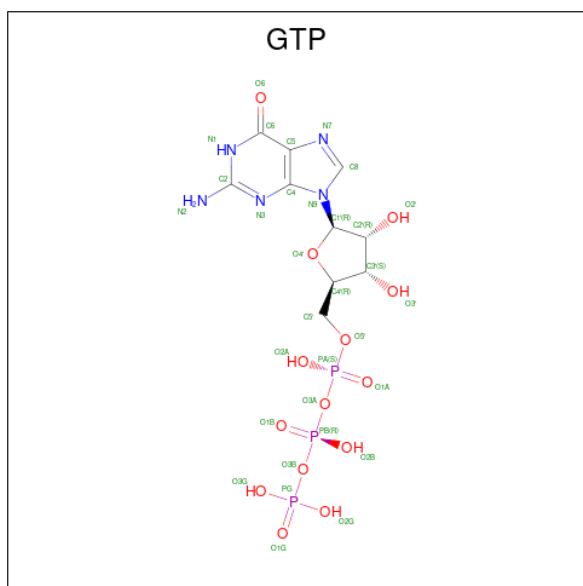
| Mol | Chain | Residues | Atoms |    |   | AltConf |
|-----|-------|----------|-------|----|---|---------|
| 90  | AA    | 1        | Total | C  | N | 0       |
|     |       |          | 14    | 10 | 4 |         |
| 90  | BA    | 1        | Total | C  | N | 0       |
|     |       |          | 14    | 10 | 4 |         |
| 90  | BA    | 1        | Total | C  | N | 0       |
|     |       |          | 14    | 10 | 4 |         |

- Molecule 91 is N-FORMYLMETHIONINE (CCD ID: FME) (formula:  $C_6H_{11}NO_3S$ ) (labeled as "Ligand of Interest" by depositor).



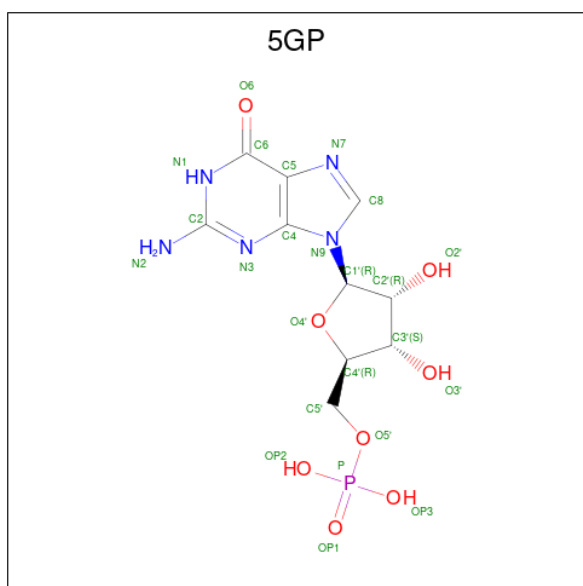
| Mol | Chain | Residues | Atoms |   |   |   |   | AltConf |
|-----|-------|----------|-------|---|---|---|---|---------|
| 91  | AV    | 1        | Total | C | N | O | S | 0       |
|     |       |          | 10    | 6 | 1 | 2 | 1 |         |

- Molecule 92 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula:  $C_{10}H_{16}N_5O_{14}P_3$ ).



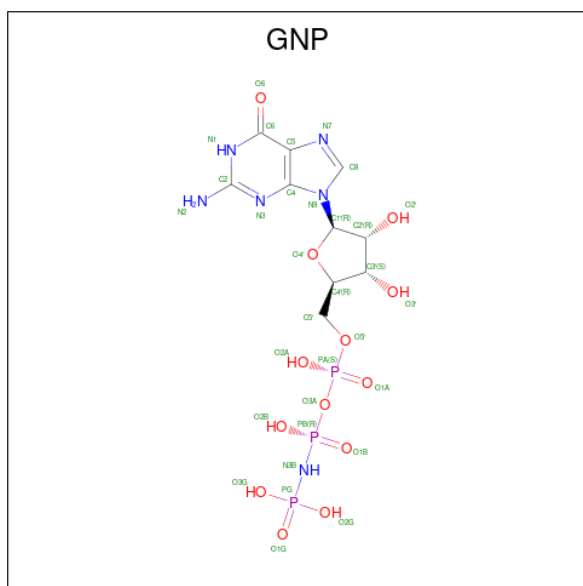
| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 92  | Ag    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 5 | 14 | 3 |         |

- Molecule 93 is GUANOSINE-5'-MONOPHOSPHATE (CCD ID: 5GP) (formula:  $C_{10}H_{14}N_5O_8P$ ).



| Mol | Chain | Residues | Atoms |    |   |   |   | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|
| 93  | BA    | 1        | Total | C  | N | O | P | 0       |
|     |       |          | 24    | 10 | 5 | 8 | 1 |         |

- Molecule 94 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (CCD ID: GNP) (formula:  $C_{10}H_{17}N_6O_{13}P_3$ ) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |    |   |    |   | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 94  | BC    | 1        | Total | C  | N | O  | P | 0       |
|     |       |          | 32    | 10 | 6 | 13 | 3 |         |

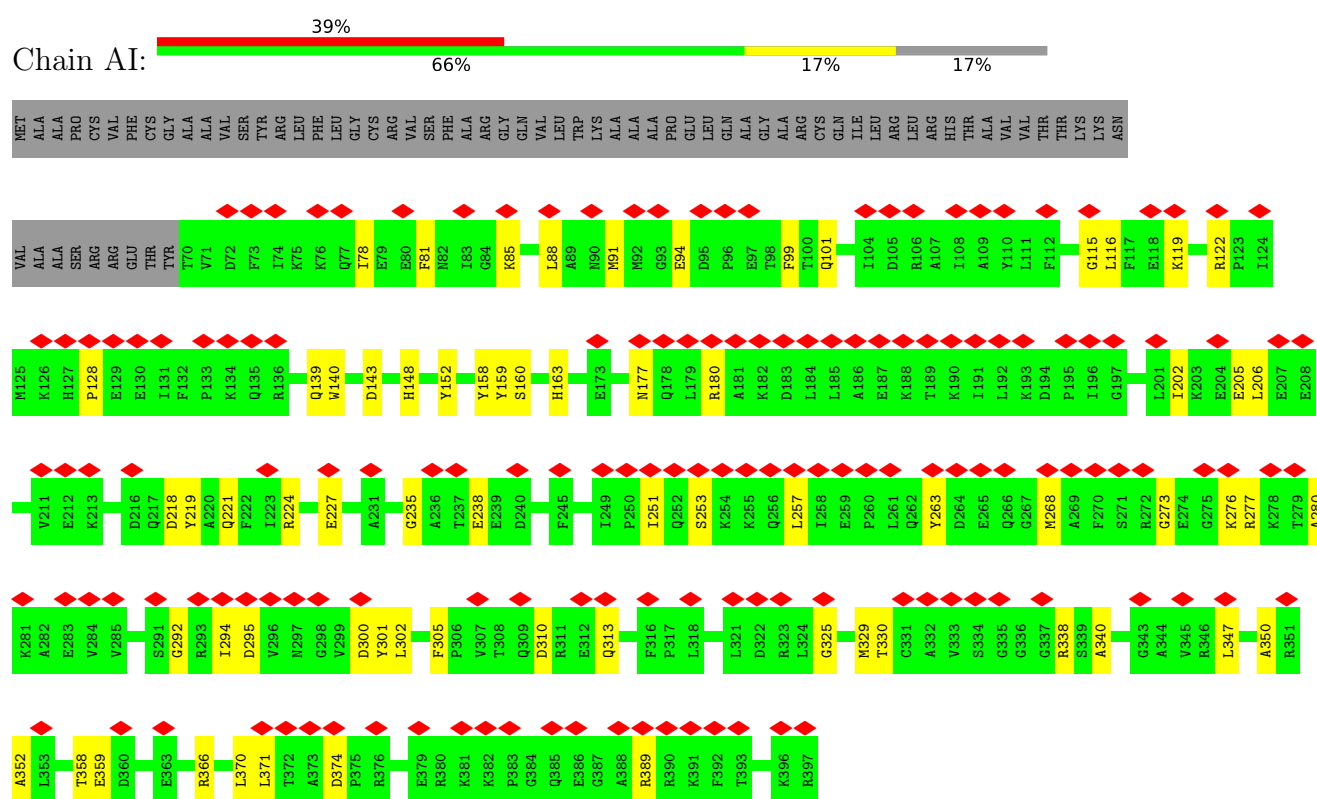
- Molecule 95 is water.

| Mol | Chain | Residues | Atoms |   | AltConf |
|-----|-------|----------|-------|---|---------|
| 95  | Ag    | 3        | Total | O | 0       |
|     |       |          | 3     | 3 |         |
| 95  | BC    | 2        | Total | O | 0       |
|     |       |          | 2     | 2 |         |

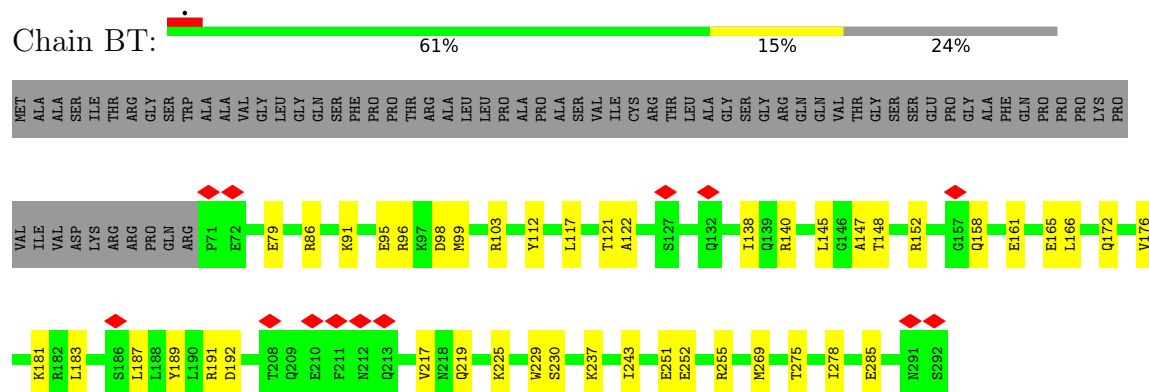
### 3 Residue-property plots

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

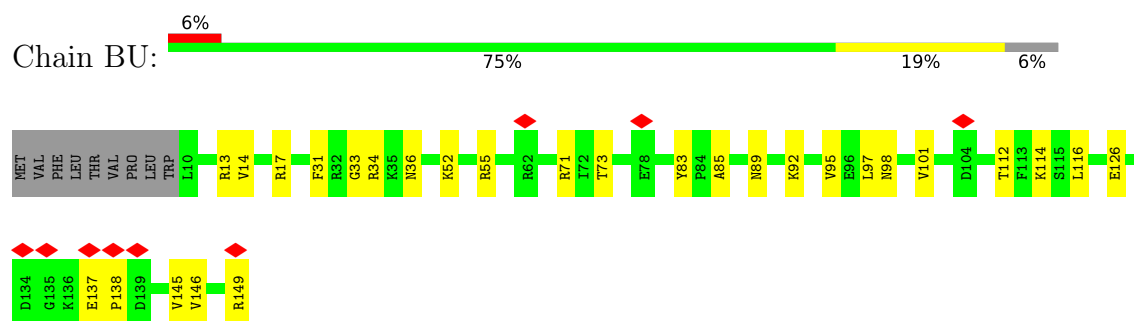
#### • Molecule 1: Uncharacterized protein



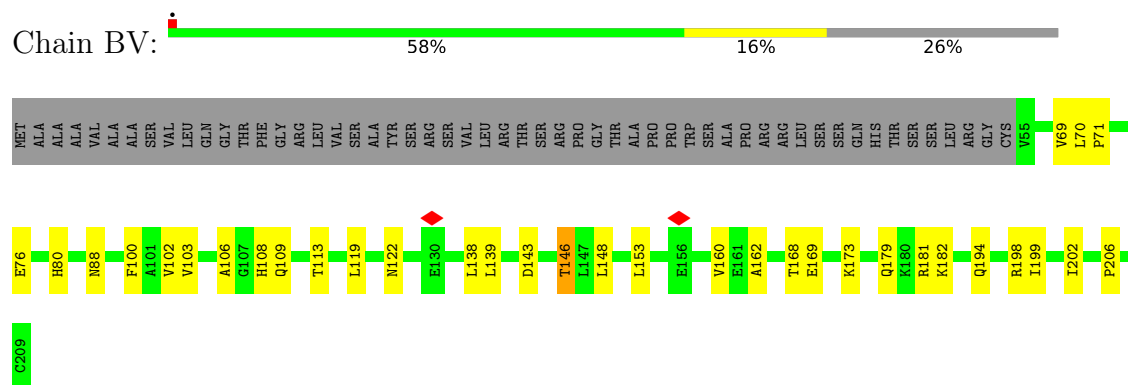
#### • Molecule 2: Mitochondrial ribosomal protein L19



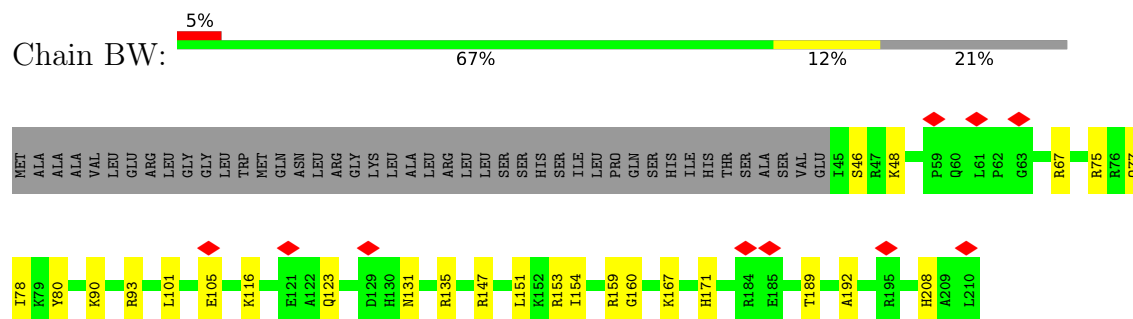
- Molecule 3: Mitochondrial ribosomal protein L20



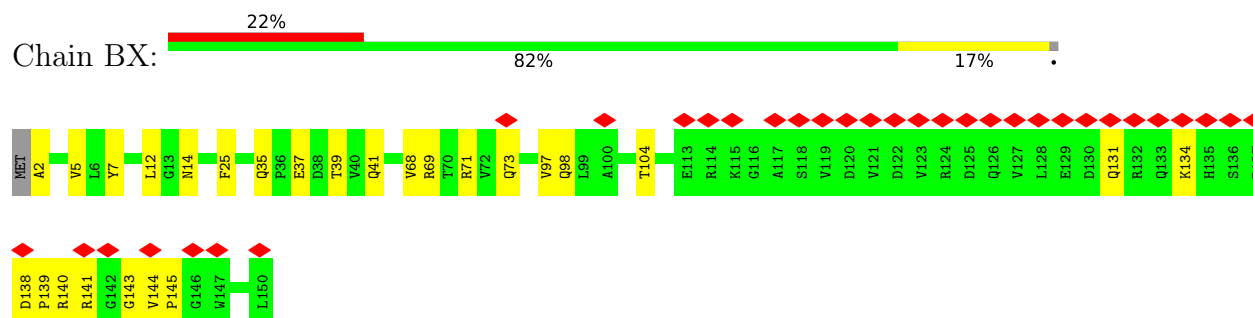
- Molecule 4: Mitochondrial ribosomal protein L21



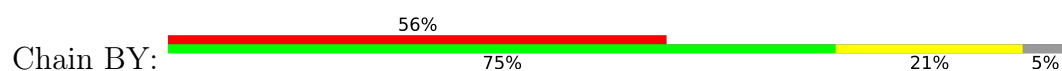
- Molecule 5: Uncharacterized protein

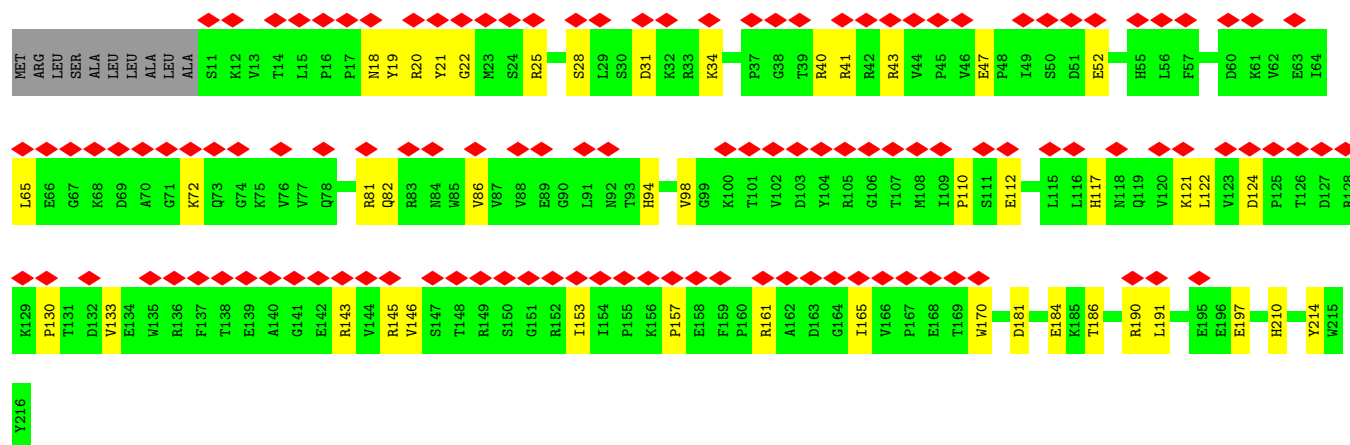


- Molecule 6: Uncharacterized protein

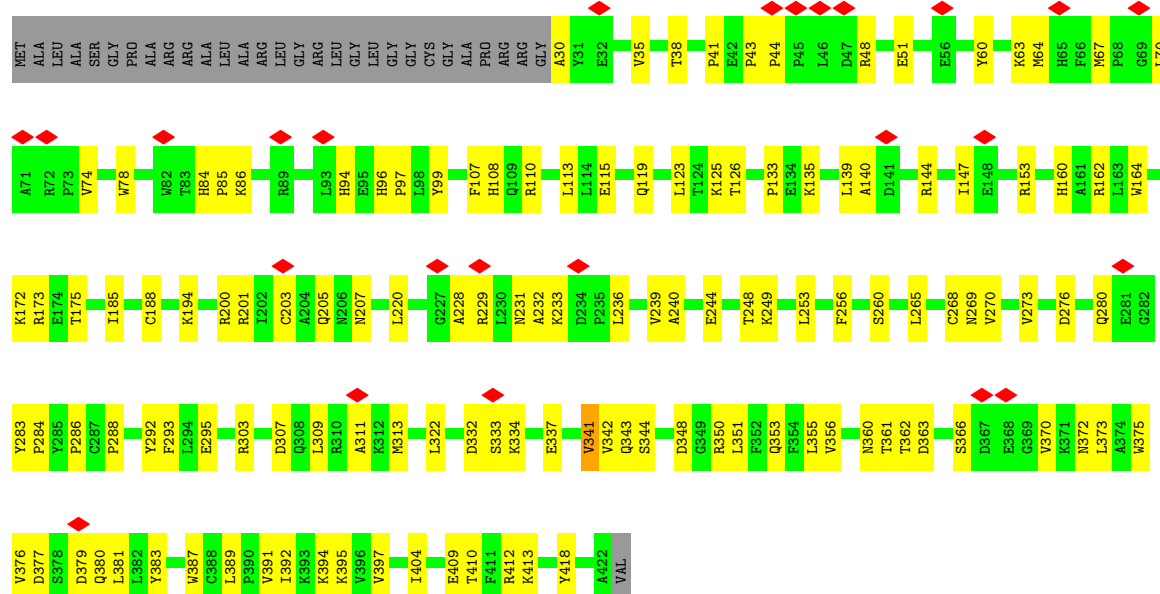


- Molecule 7: Uncharacterized protein

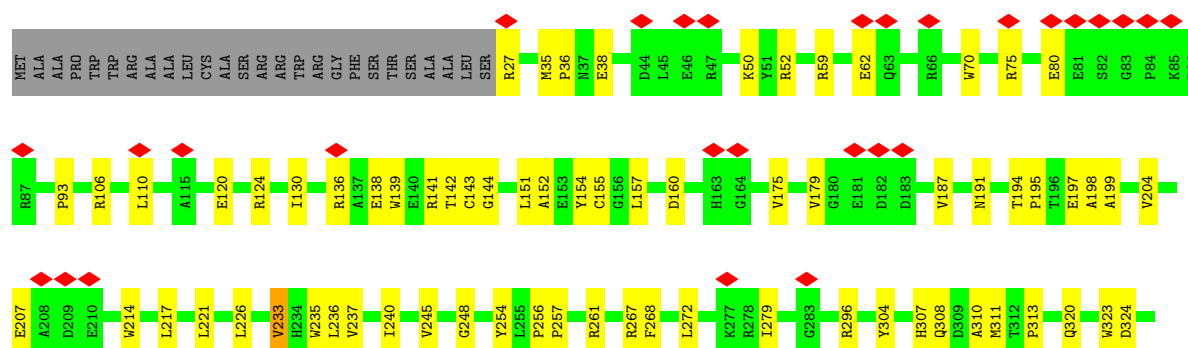
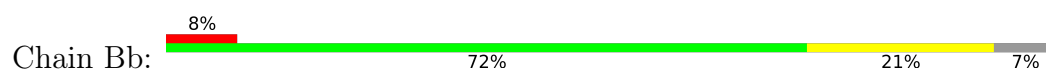




• Molecule 8: Mitochondrial ribosomal protein L37

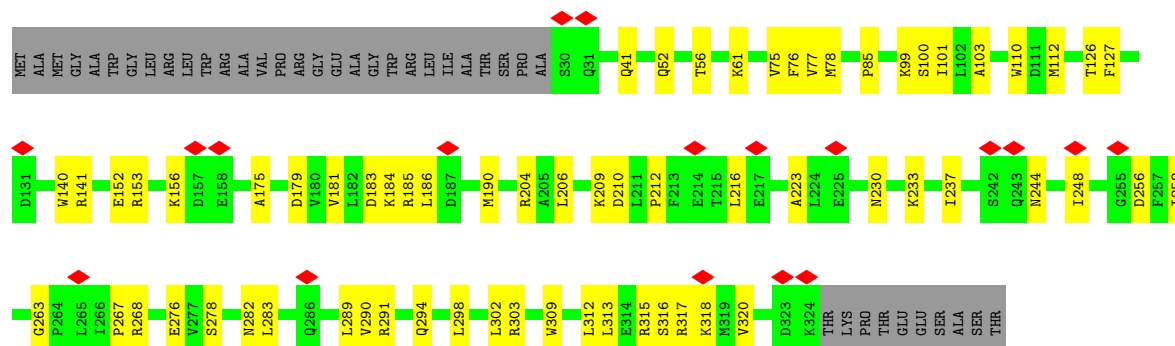


• Molecule 9: Mitochondrial ribosomal protein L38

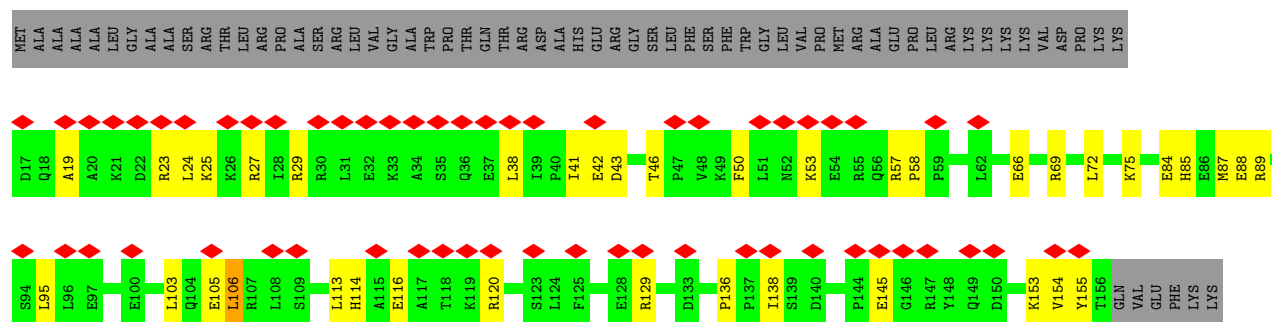




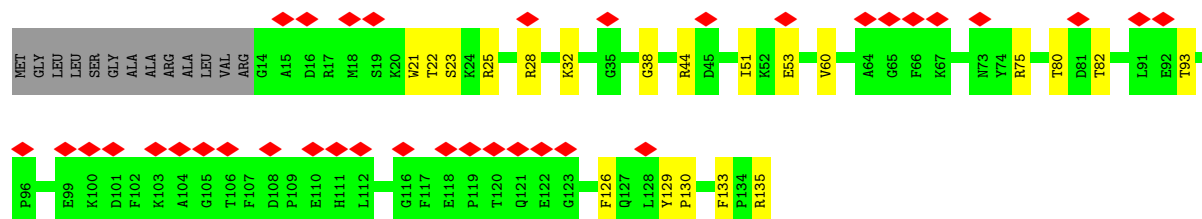
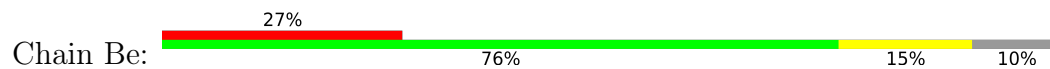
- Molecule 10: Mitochondrial ribosomal protein L39



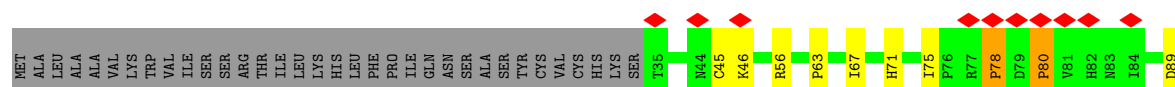
- Molecule 11: Uncharacterized protein

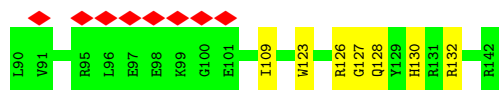


- Molecule 12: Mitochondrial ribosomal protein L41

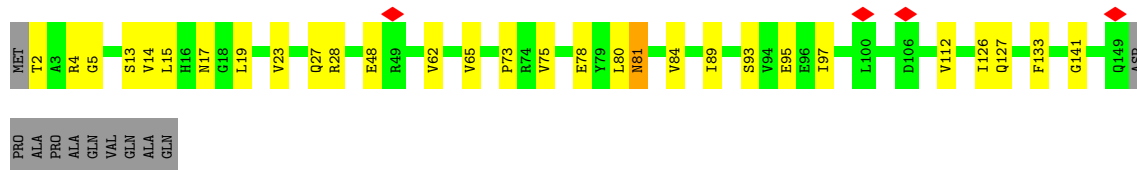
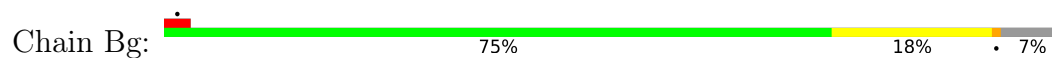


- Molecule 13: Uncharacterized protein

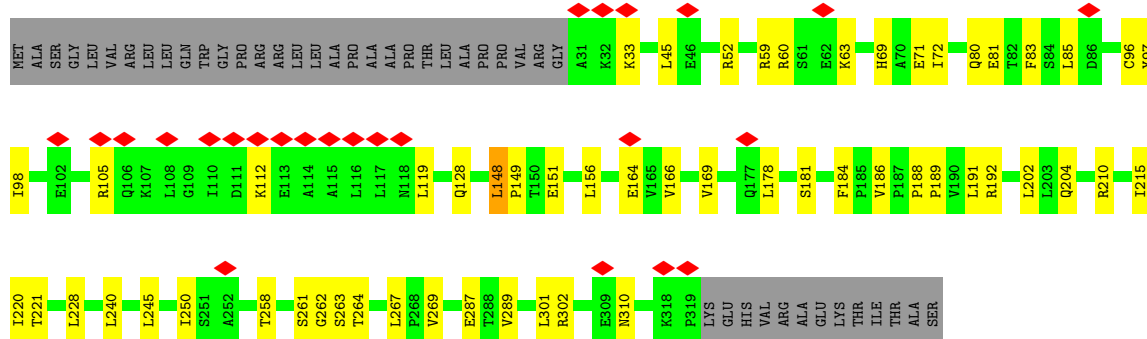
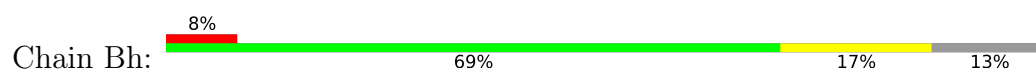




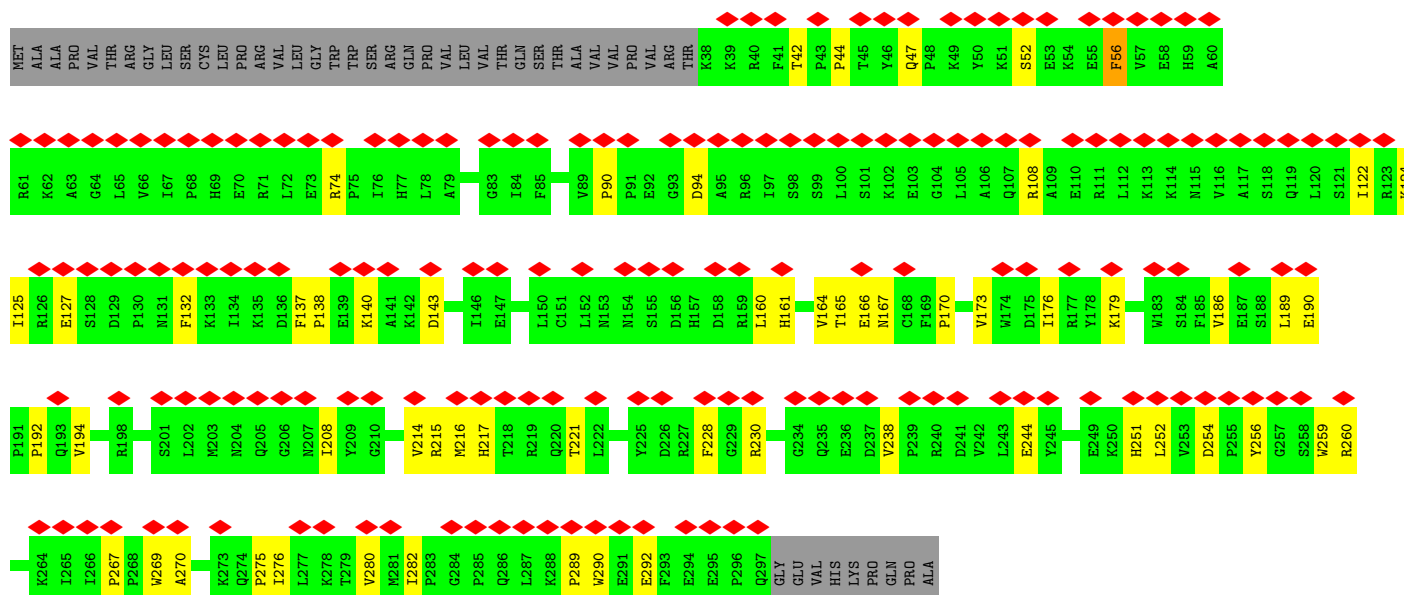
• Molecule 14: Mitochondrial ribosomal protein L43



• Molecule 15: Uncharacterized protein



• Molecule 16: Mitochondrial ribosomal protein L45



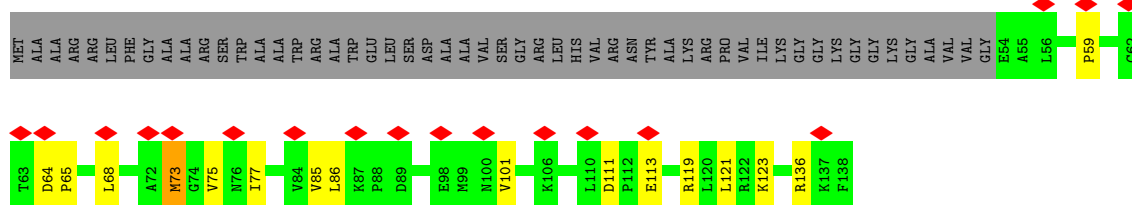
Chain B<sub>i</sub>: 



Chain Bm:



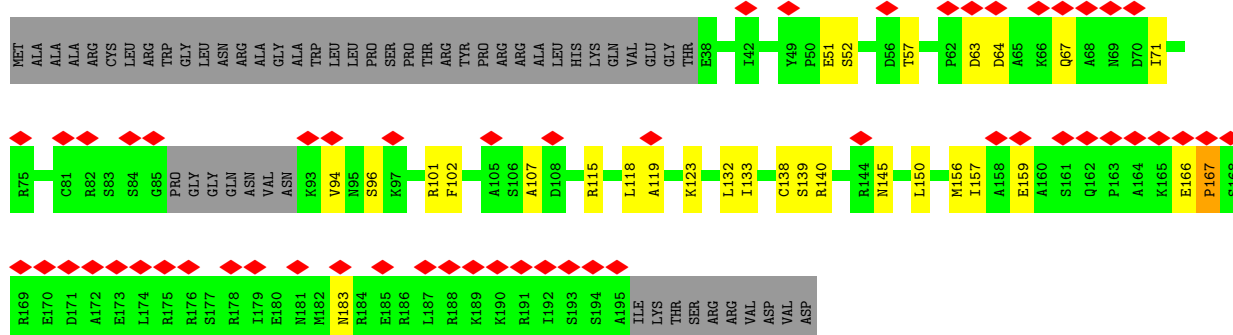
- Molecule 24: Uncharacterized protein



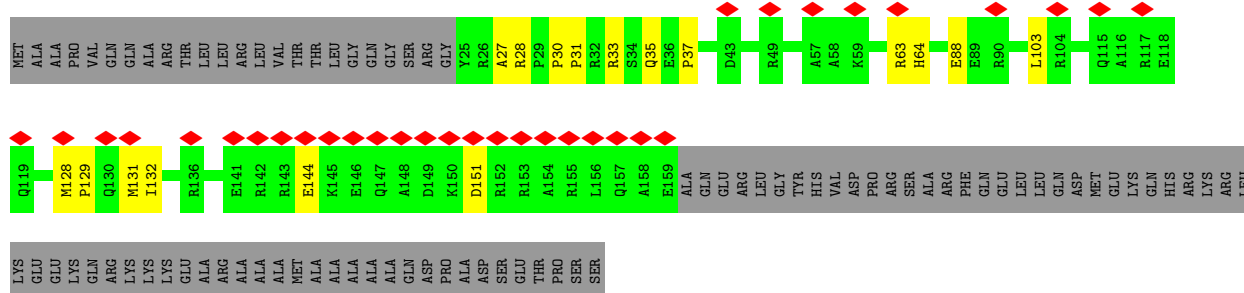
- Molecule 25: Mitochondrial ribosomal protein L57



- Molecule 26: Uncharacterized protein



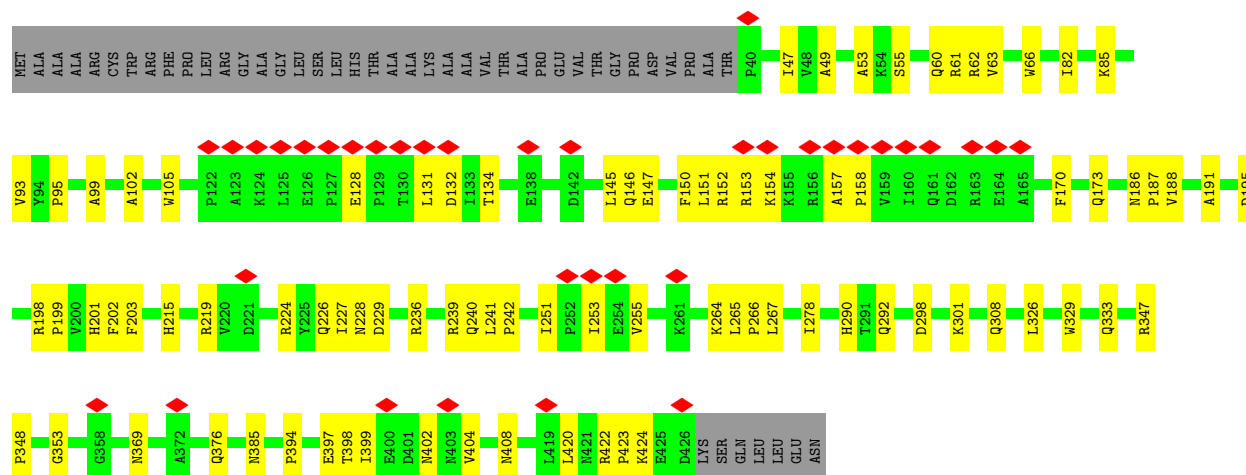
- Molecule 27: Uncharacterized protein



- Molecule 28: Mitochondrial ribosomal protein L27



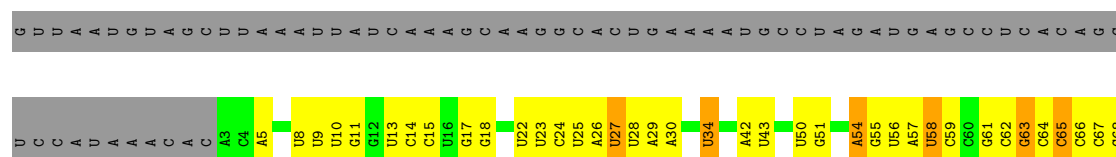
- Molecule 29: 39S ribosomal protein S30, mitochondrial



- Molecule 30: Mitochondrial ribosomal protein S18A



- Molecule 31: 12S rRNA











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[illegible]

- Molecule 31: 12S rRNA

Chain BA:  . . .

91%











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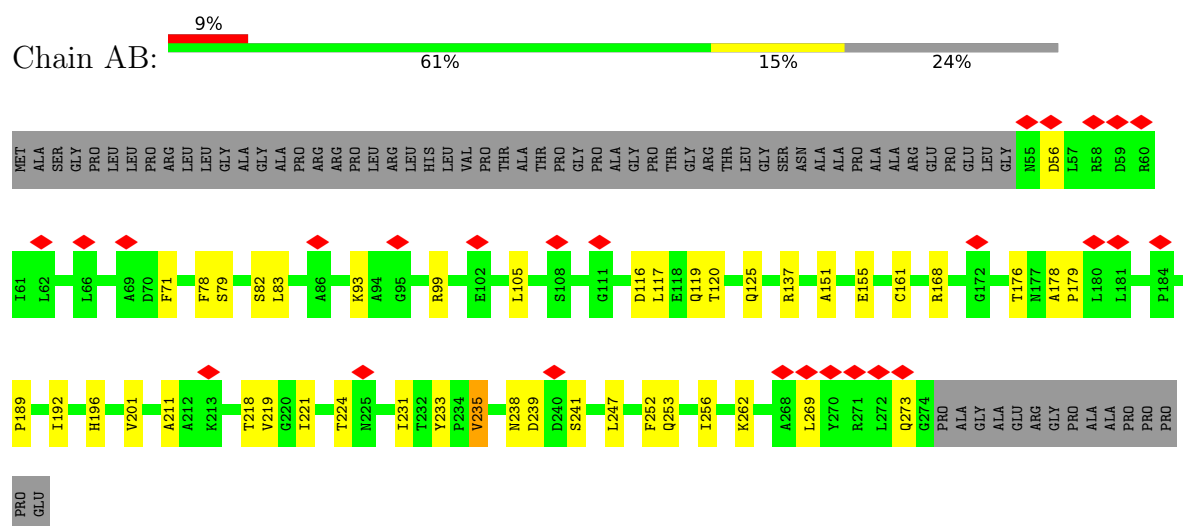
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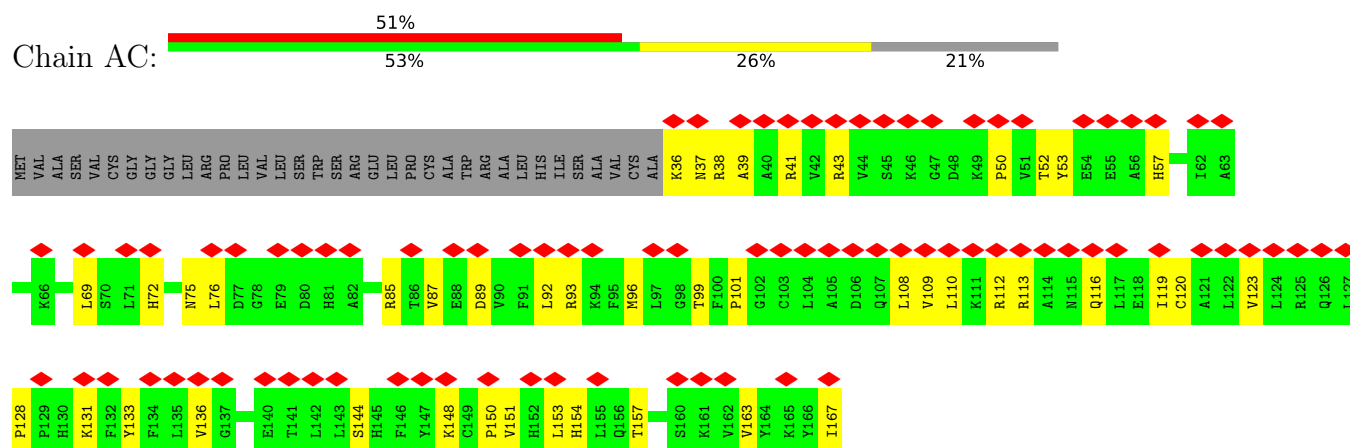
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- Molecule 32: Mitochondrial ribosomal protein S2

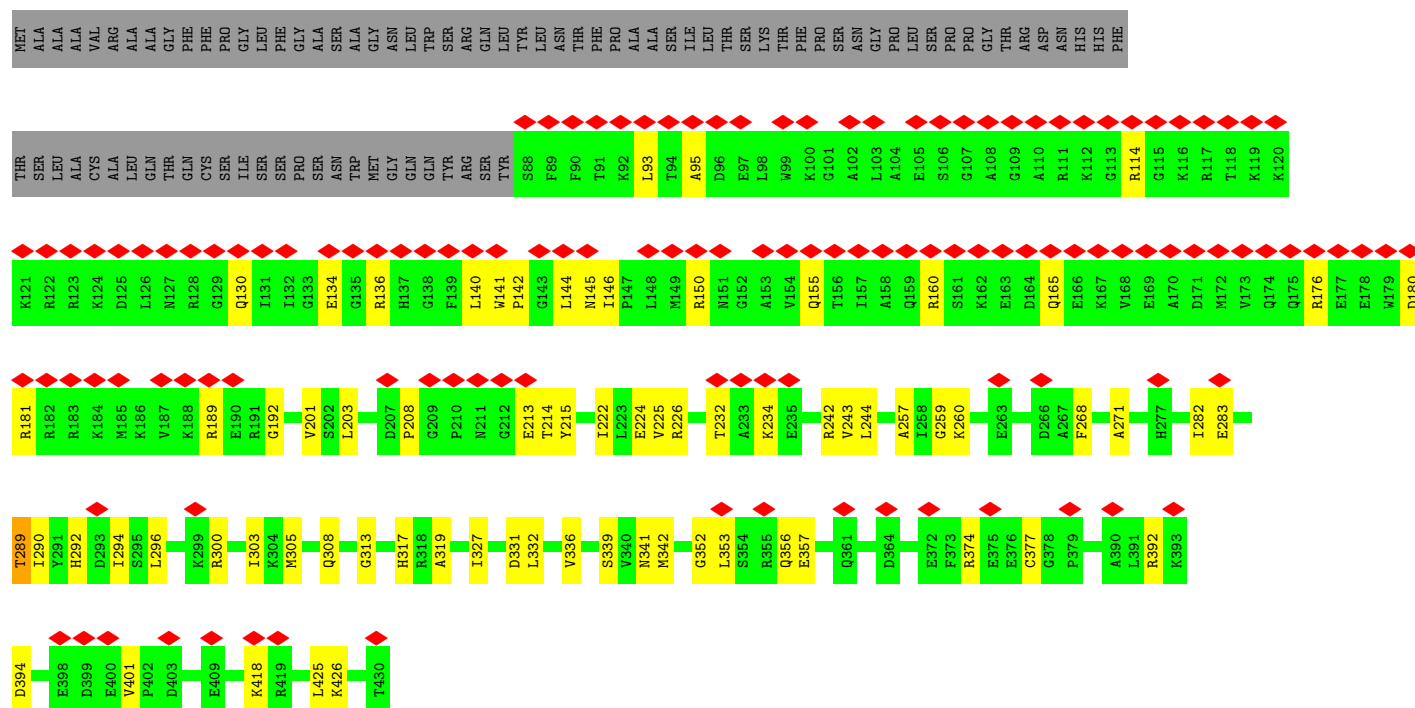


- Molecule 33: Mitochondrial ribosomal protein S24

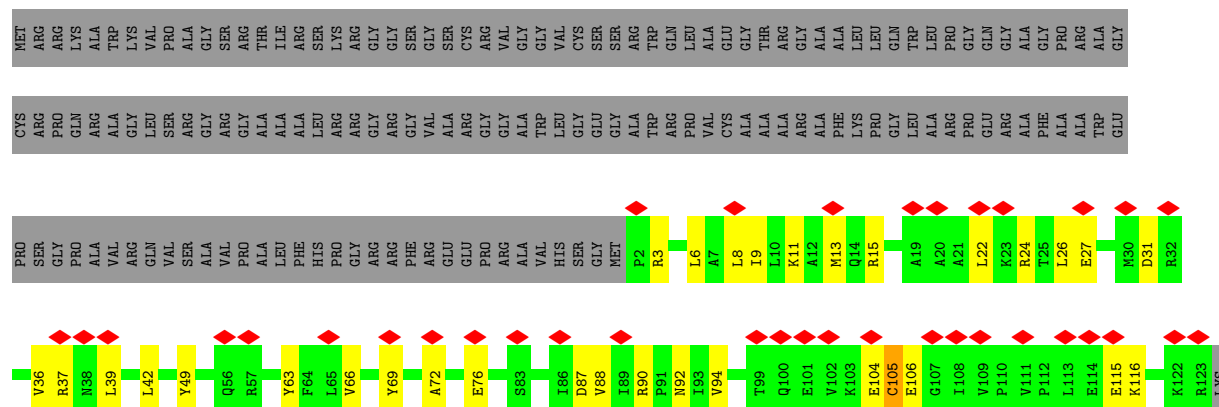
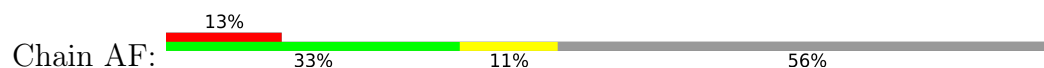


- Molecule 34: Mitochondrial ribosomal protein S5

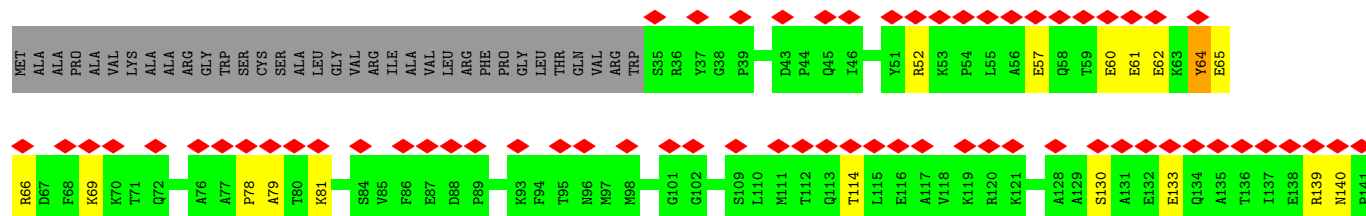


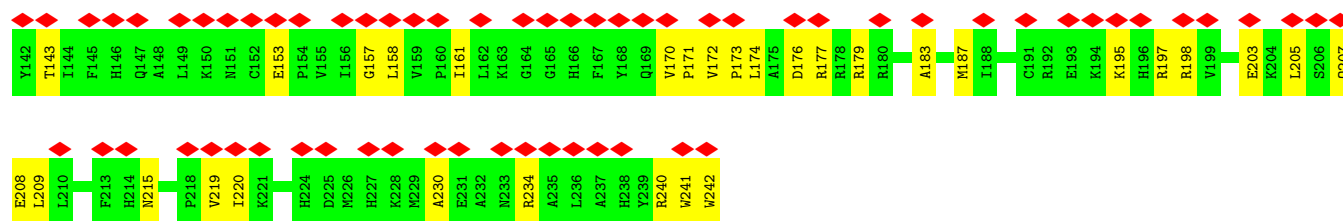


• Molecule 35: Uncharacterized protein

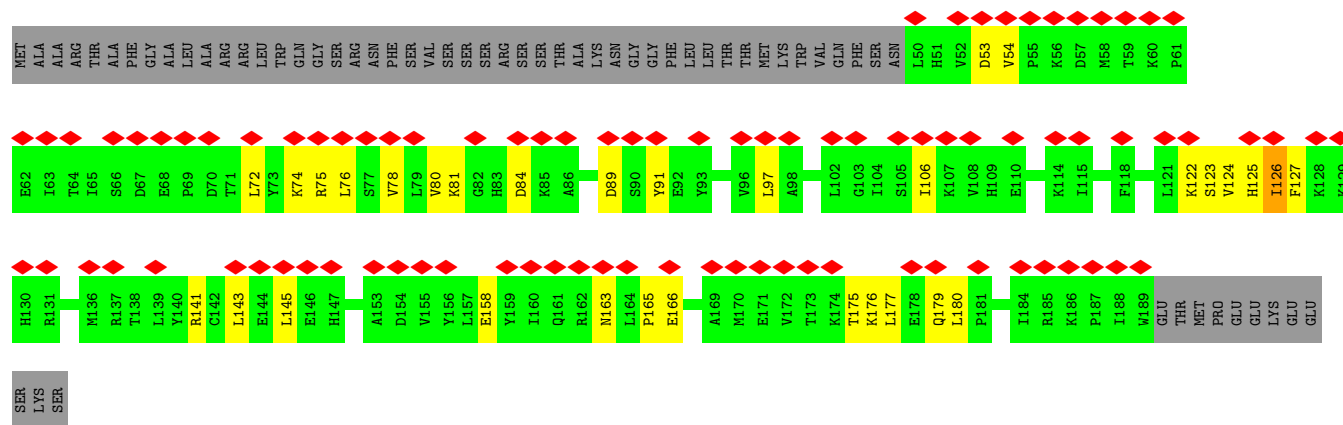


• Molecule 36: Mitochondrial ribosomal protein S7

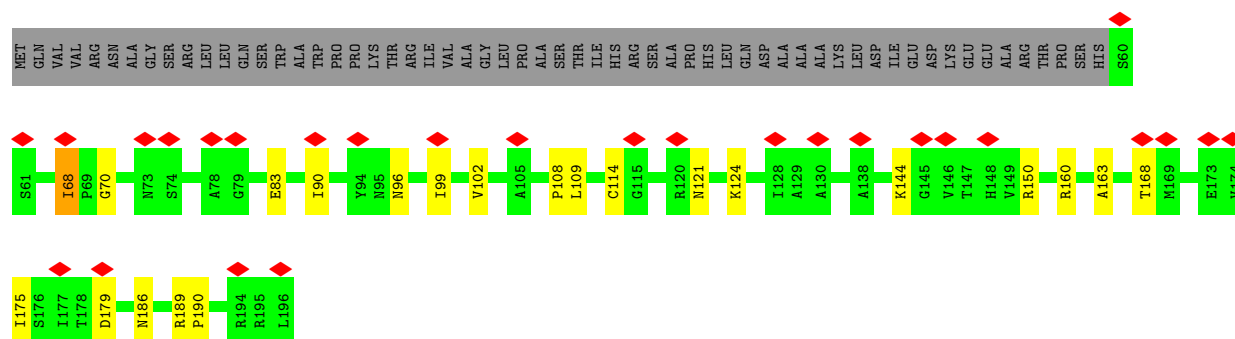




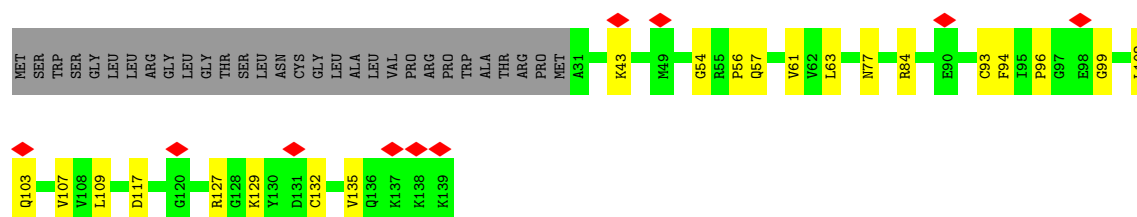
• Molecule 37: Mitochondrial ribosomal protein S10



• Molecule 38: uS11m

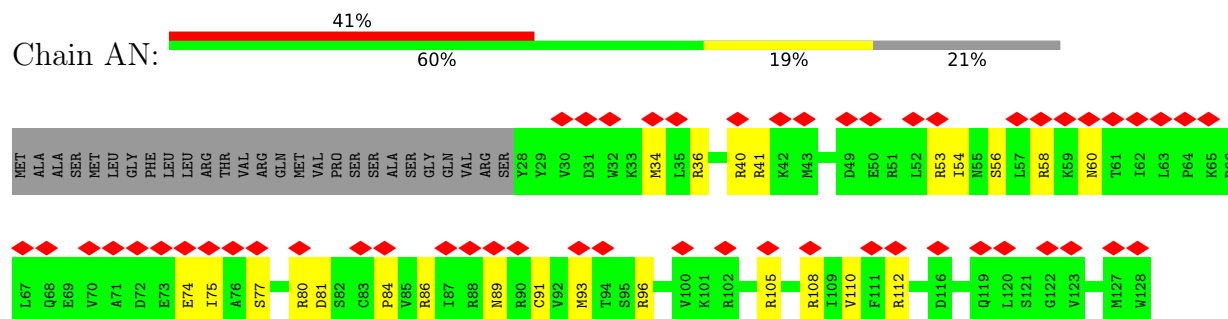


• Molecule 39: Mitochondrial ribosomal protein S12



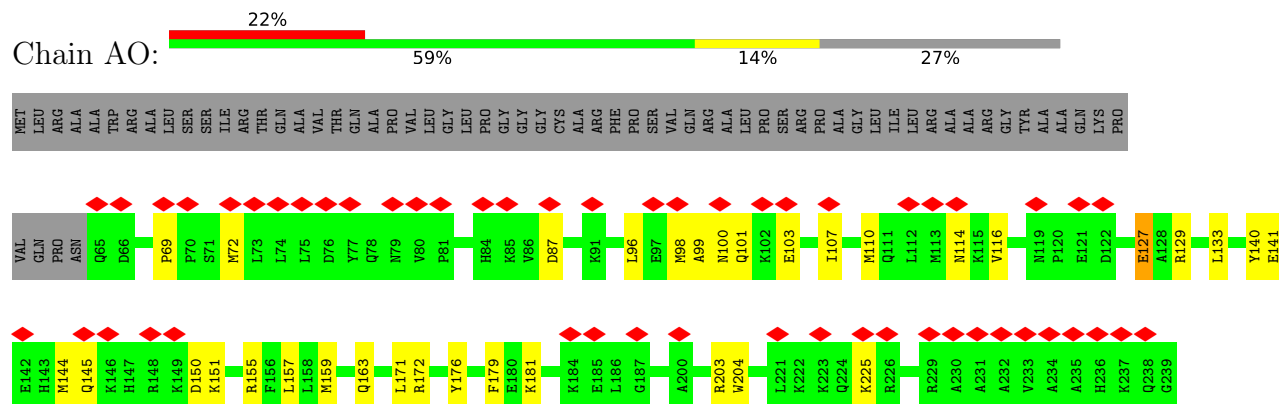
## • Molecule 40: Mitochondrial ribosomal protein S14

Chain AN:



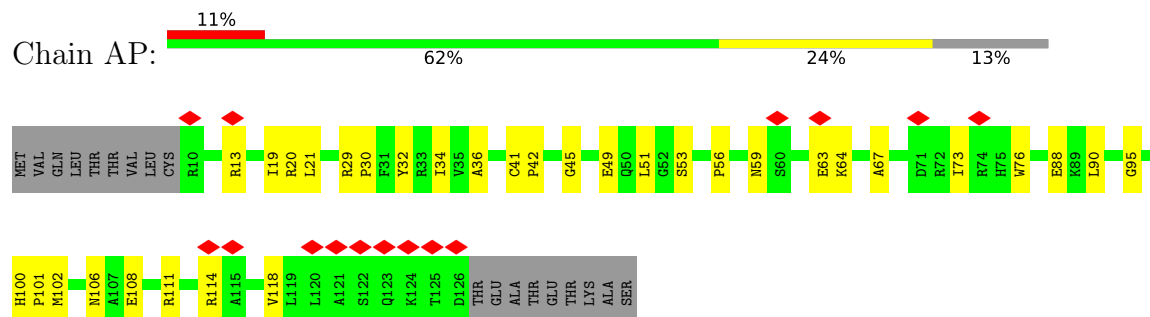
## • Molecule 41: uS15m

Chain AO:



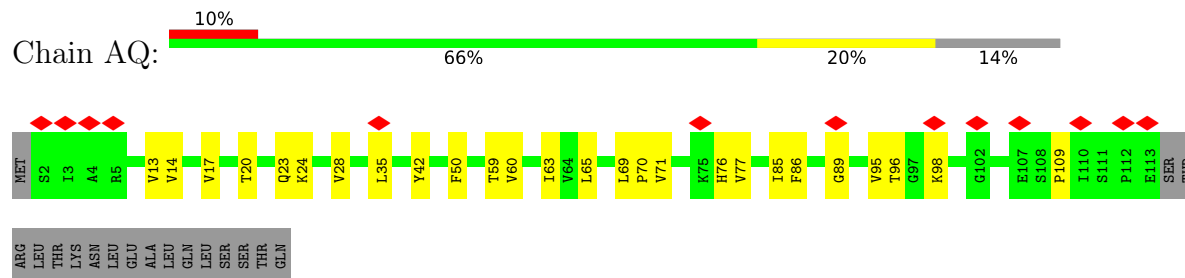
## • Molecule 42: 28S ribosomal protein S16, mitochondrial

Chain AP:



## • Molecule 43: uS17m

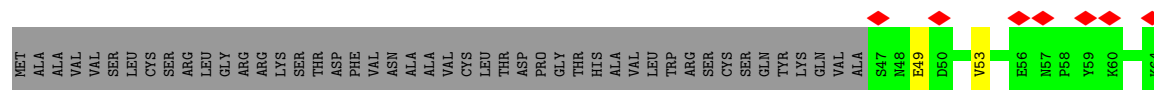
Chain AQ:



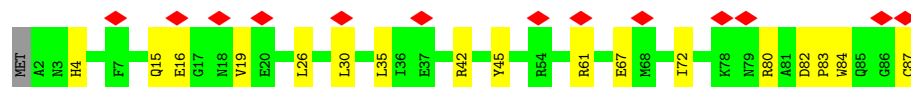
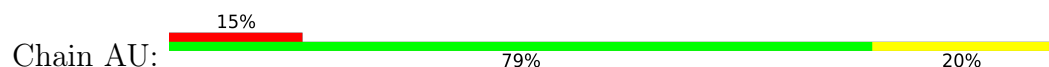
## • Molecule 44: Mitochondrial ribosomal protein S18C

Chain AR:

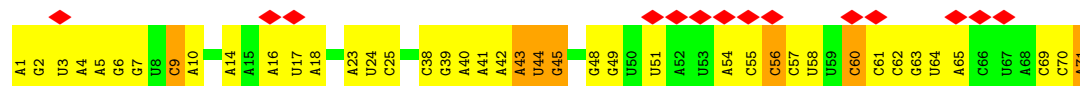
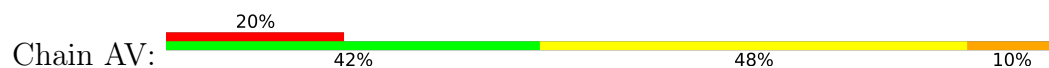




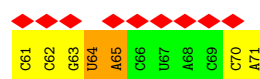
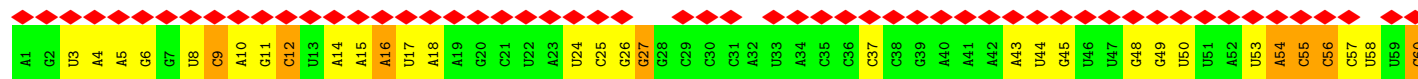
- Molecule 45: bS21m



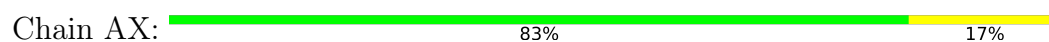
- Molecule 46: tRNAMet



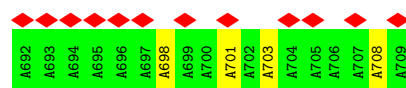
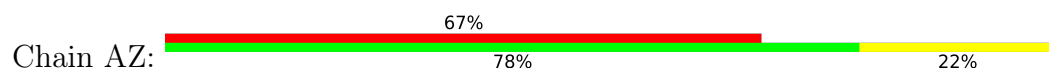
- Molecule 46: tRNAMet



- Molecule 47: mRNA

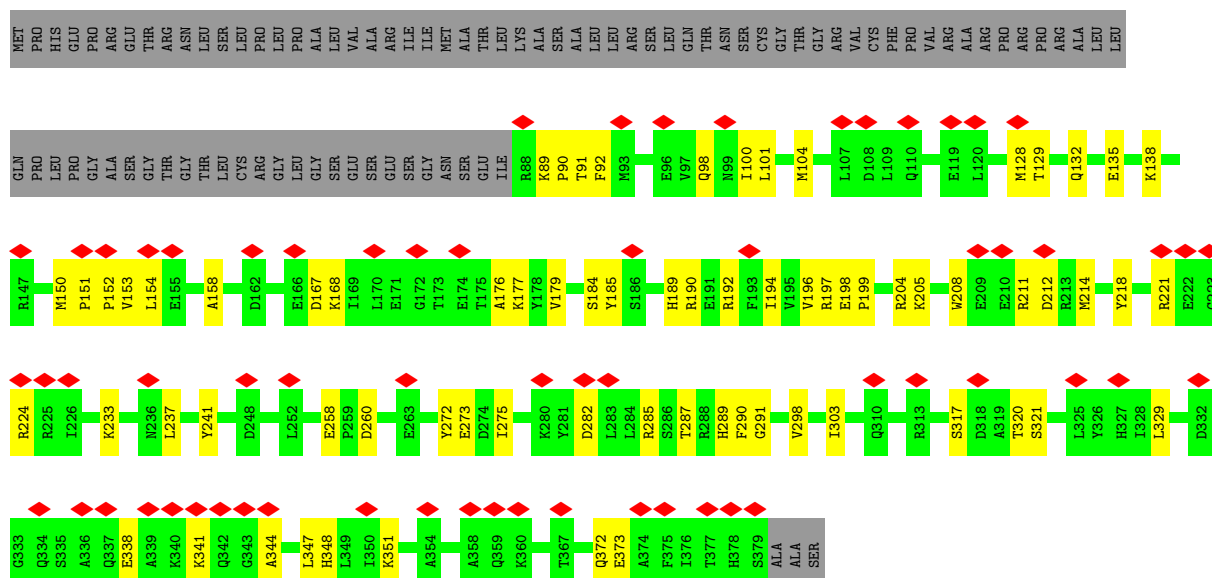


- Molecule 48: unknown peptide

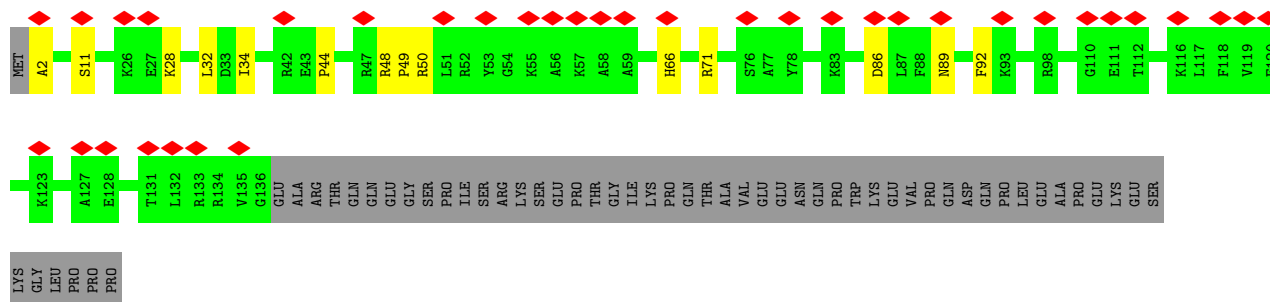


- Molecule 49: Mitochondrial ribosomal protein S22

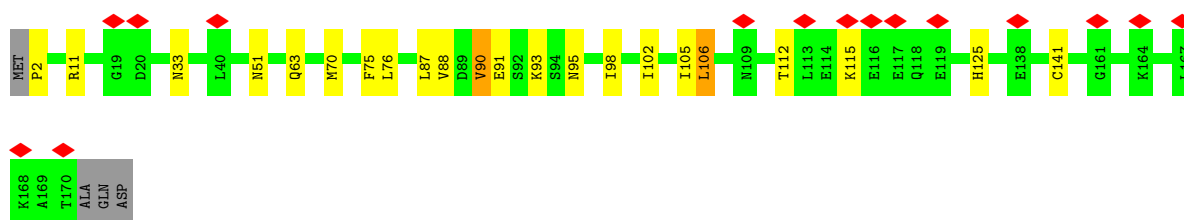
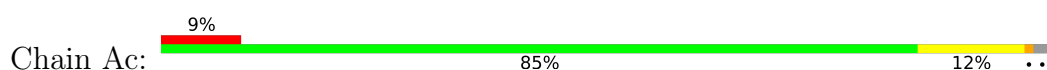




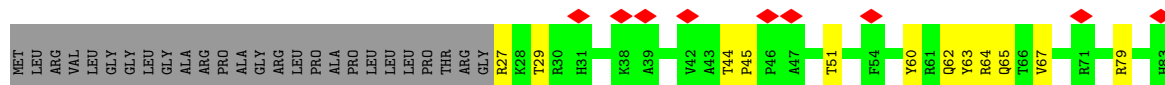
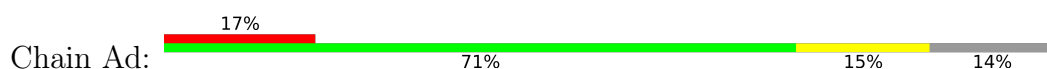
• Molecule 50: mS23

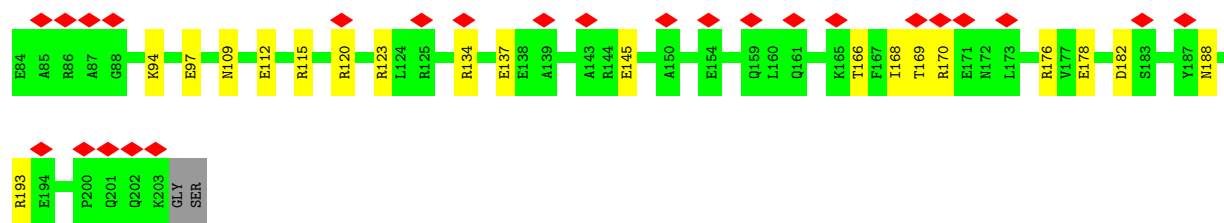


• Molecule 51: Mitochondrial ribosomal protein S25

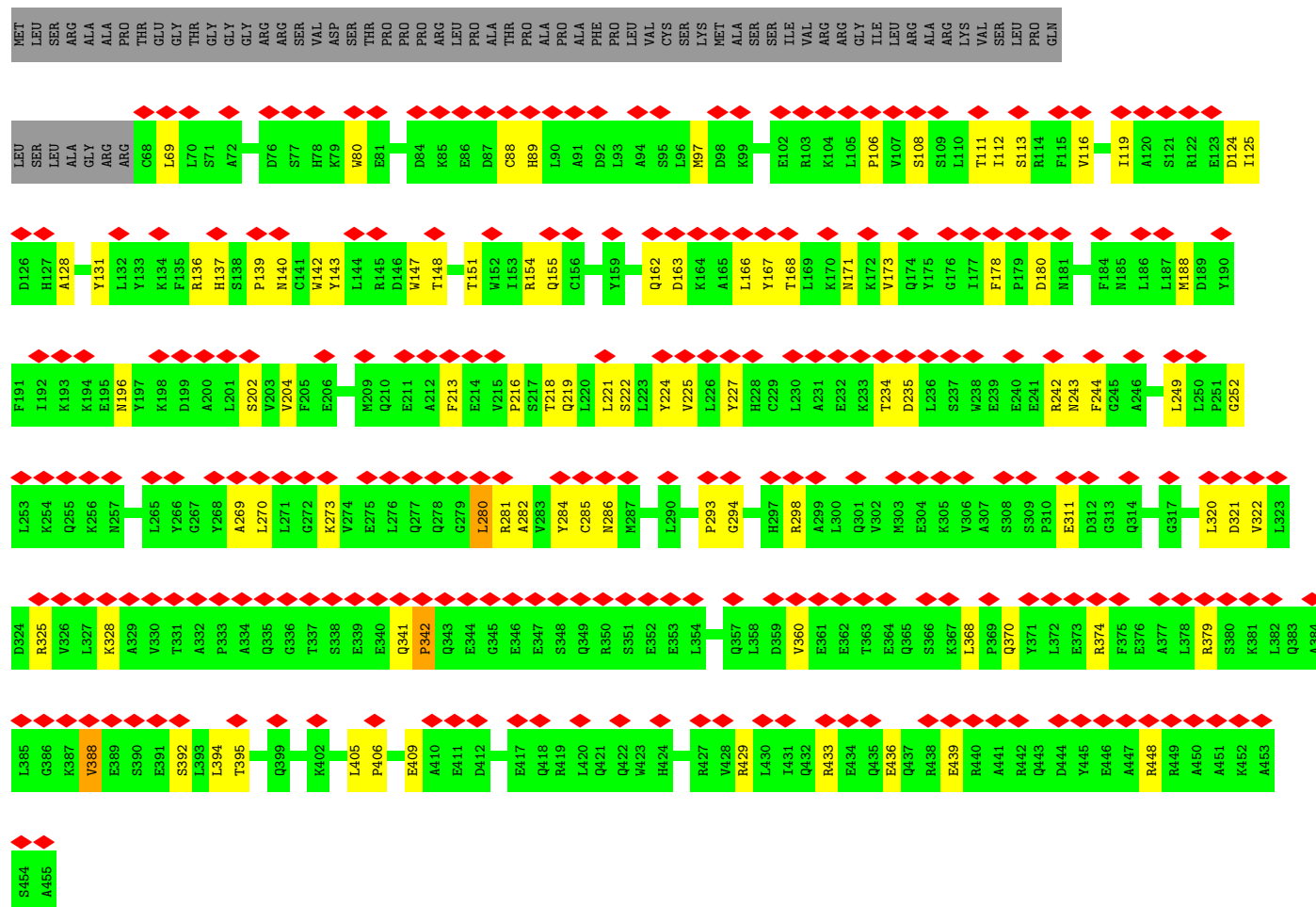


• Molecule 52: Mitochondrial ribosomal protein S26

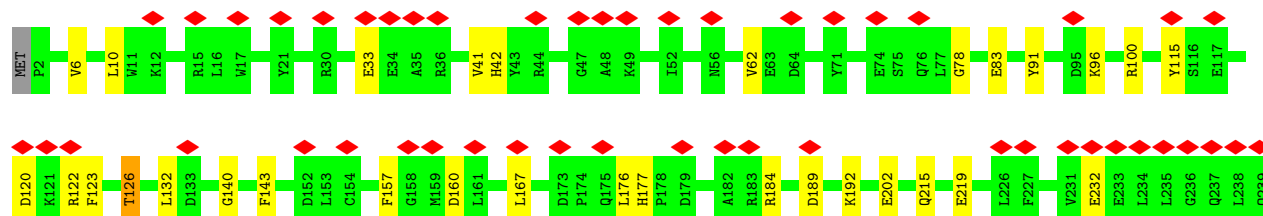
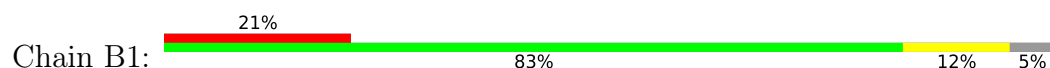




• Molecule 53: Mitochondrial ribosomal protein S27

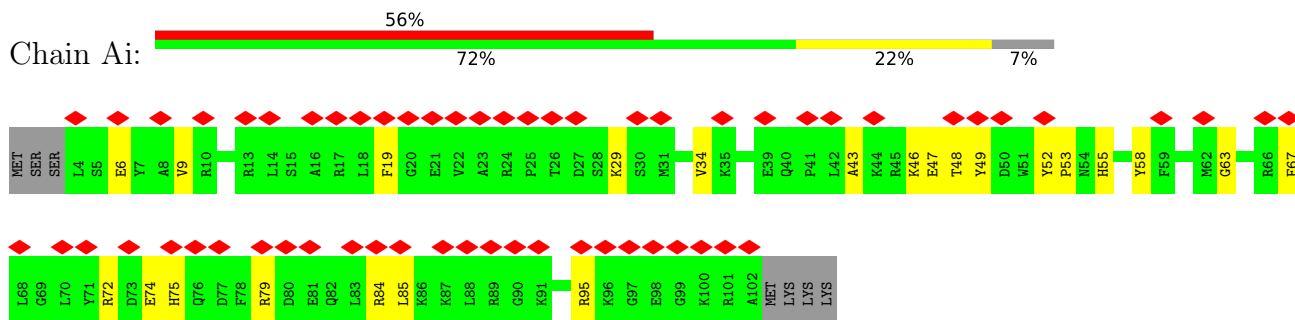


• Molecule 54: Mitochondrial ribosomal protein L28

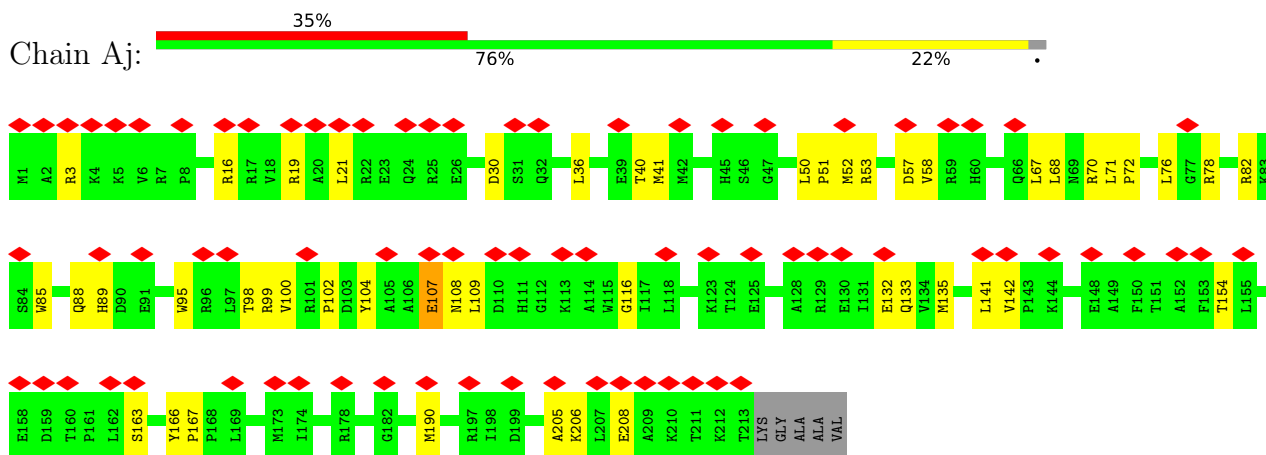




- Molecule 58: mS33



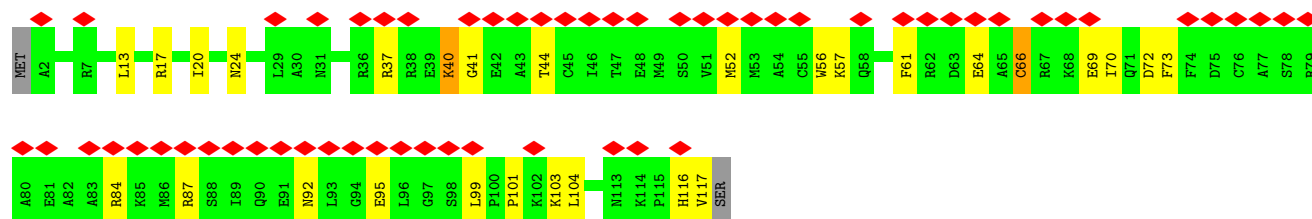
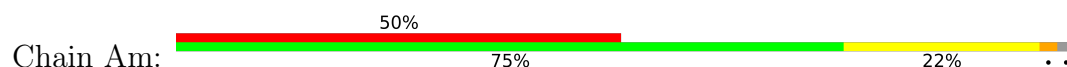
- Molecule 59: mS34



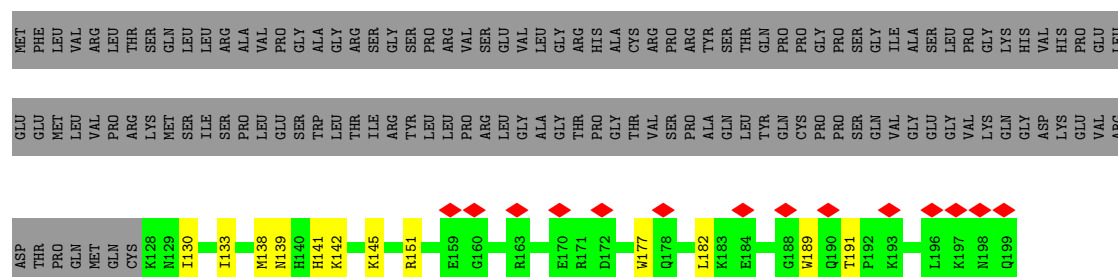
- Molecule 60: Mitochondrial ribosomal protein S35



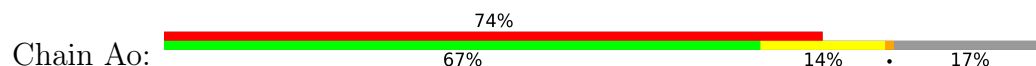
- Molecule 61: mS37

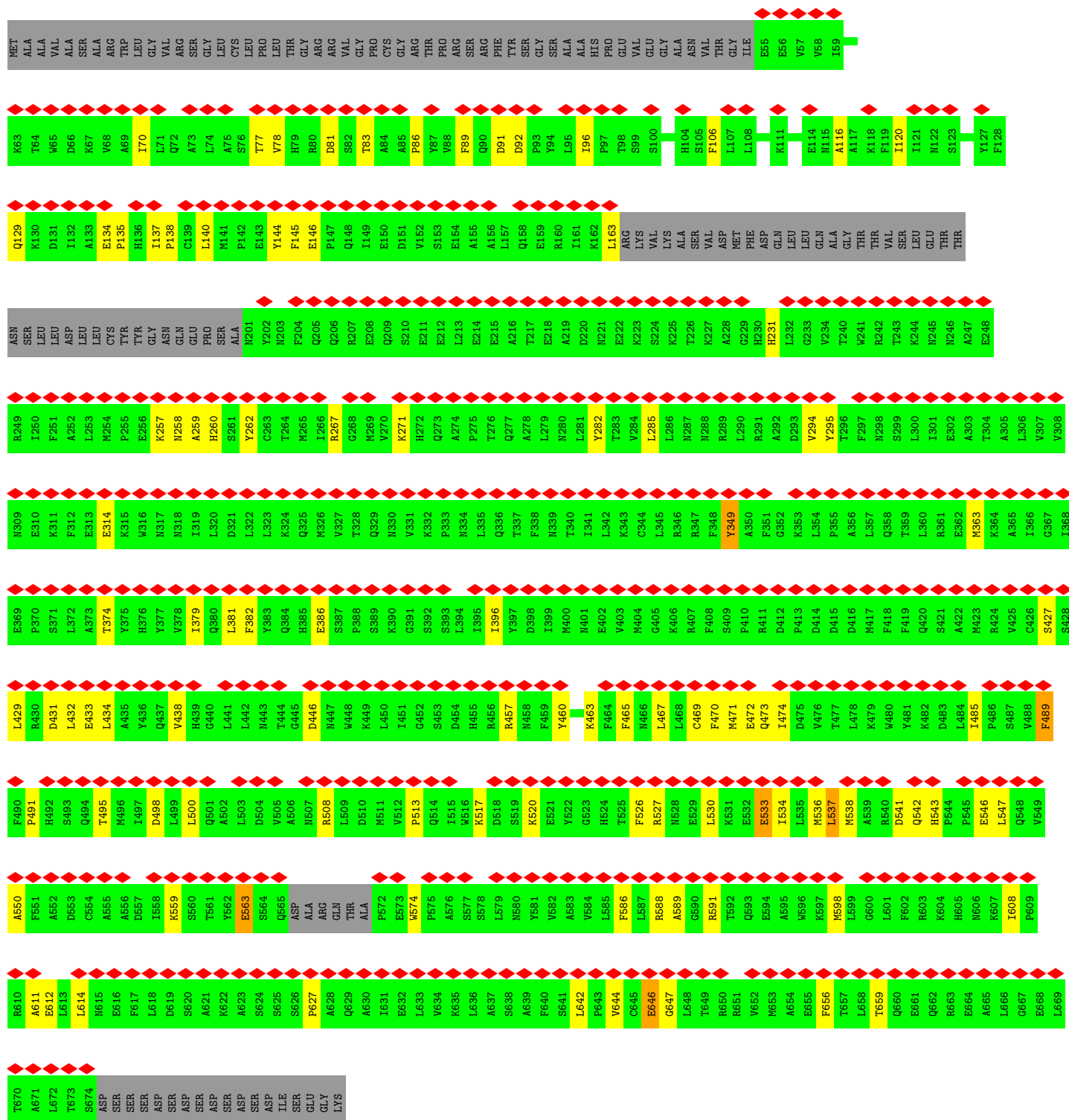


- Molecule 62: Aurora kinase A interacting protein 1

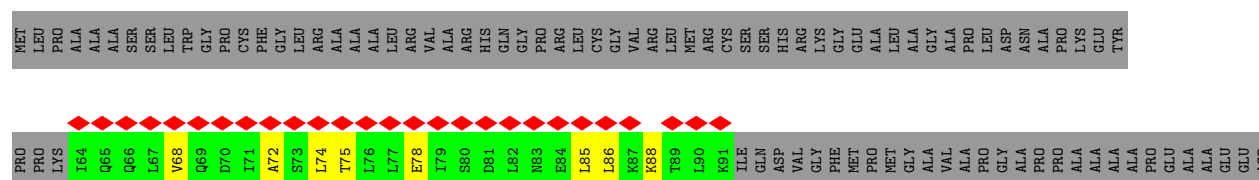


- Molecule 63: mS39

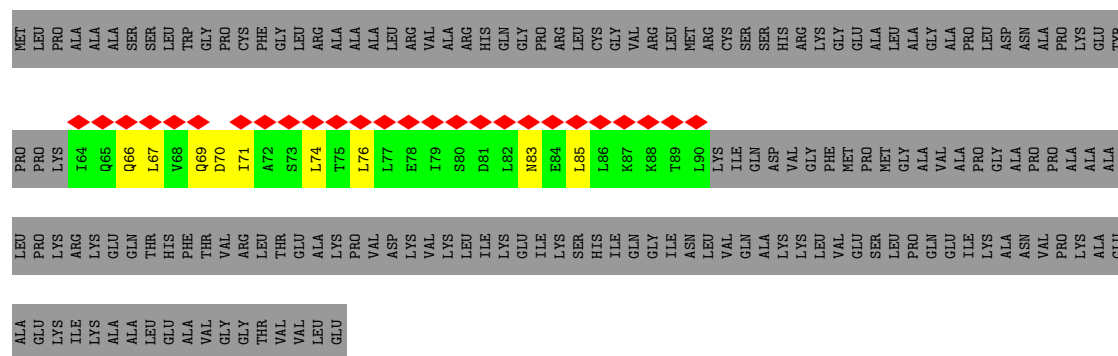




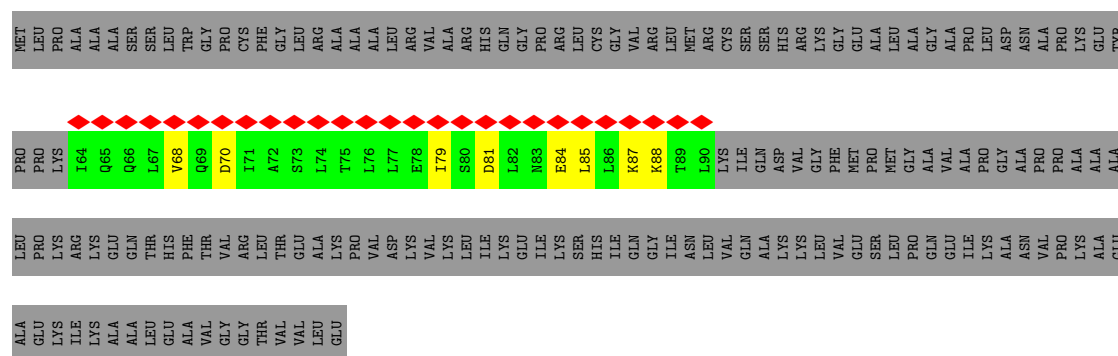
• Molecule 64: 28S ribosomal protein S18b, mitochondrial



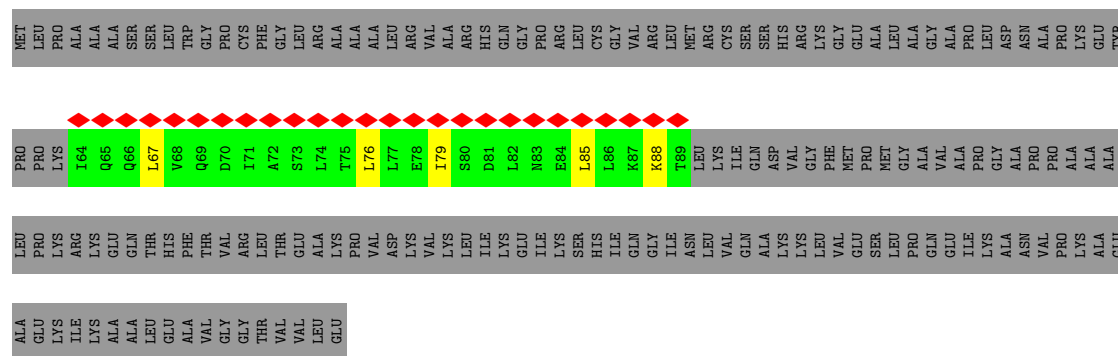
- Molecule 65: Mitochondrial ribosomal protein L12



- Molecule 65: Mitochondrial ribosomal protein L12



- Molecule 65: Mitochondrial ribosomal protein L12



- Molecule 65: Mitochondrial ribosomal protein L12



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

PRO PRO LYS ILE GLN LEU VAL GLN ASP ILE ALA SER LEU THR LEU ARG ALA ALA ALA ALA VAL ARG HIS LYS VAL GLY LEU ALA PRO ALA ASP ASN ALA PRO LYS TYR

LEU PRO LYS ARG LYS GLN THR H129 F130 F131 V132 R133 L134 T135 E136 A137 K138 P139 V140 D141 K142 V143 K144 L145 T146 K147 E148 I149 K150 S151 H152 I153 Q154 G155 I156 M157 L158 V159 Q160 A161 K162 K163 V165 E166 S167 L168 P169 Q170 E171 I172 K173 A174 M175 V176 P177 K178 A179 E180

• Molecule 66: Mitochondrial ribosomal protein L47



MET ALA ALA ALA GLY LEU VAL PHE CYS ARG ARG VAL SER ALA ALA LYS CYS ARG LEU ILE ARG PRO GLN ALA PRO PRO SER SER THR CYS ARG PHE SER PRO SER LEU LEU PRO LYS ASN THR PRO ASN VAL THR SER PHE HIS GLN PHE ILE PHE HIS THR

PHE SER ARG G65 K74 Q90 Q91 L92 S95 S96 D99 L100 R111 M128 P131 L144 D153 R156 L157 L158 G161 Q162 E163 R172 W190 R200 A203 M204 P205 R226 S227 L228 K231 E238 K239 F240 P241 H242 L243 SER GLU

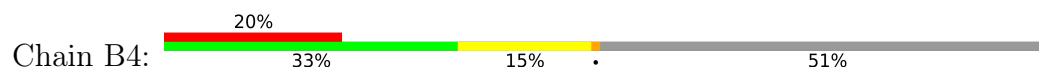
• Molecule 67: Uncharacterized protein



HIS PRO PRO ARG GLN ASP PHE LEU VAL ARG ARG GLN PRO HIS ARG ASN ARG THR VAL THR LYS GLY MET GLU SER LEU ILE CYS ASP TRP ILE ARG K35 R38 S39 R40 S49 P50 E51 D52 H64 K65 L66 I68 V69 R70 R71 I72 K73 S74 R77 R78

K83 M88 K93 T96 K101 N102 I103 P104 S105 V106 A107 K109 V113 K114 I117 R118 I119 K120 P121 L122 E132 D133 M134 T137 R148 L151 N152 PRO ALA ASN GLN GLU ALA ARG LYS

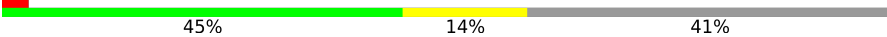
• Molecule 68: Uncharacterized protein

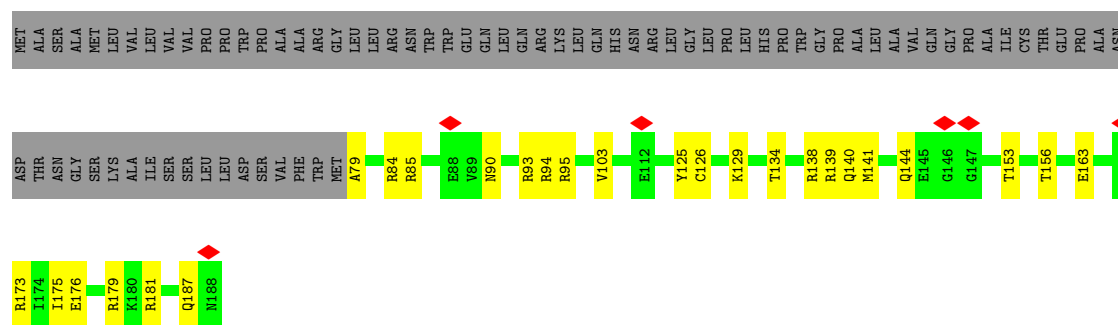


MET ALA ALA LYS GLY SER LEU ARG ARG LEU TRP GLN ARG VAL VAL THR GLY ALA ALA PRO GLU SER GLU CYS ARG HIS LEU TYR THR SER SER TRP ARG D35 R38 L41 T42 R43 L44 H45 R46 Q47 T48 A50 Y53 Y57 V58 K59 Q60 D61 G62 S63 T64 I65

R68 Y69 E70 P72 R73 M78 P79 V80 D81 L82 D83 S84 L85 S86 P87 E88 E89 R90 R91 A92 R93 F94 R95 K96 ARG GLU ALA LYS PHE LYS GLU LYS LYS R43 T42 R43 L44 H45 R46 Q47 T48 A50 Y53 Y57 V58 K59 Q60 D61 G62 S63 T64 I65

• Molecule 69: Uncharacterized protein

Chain B5: 



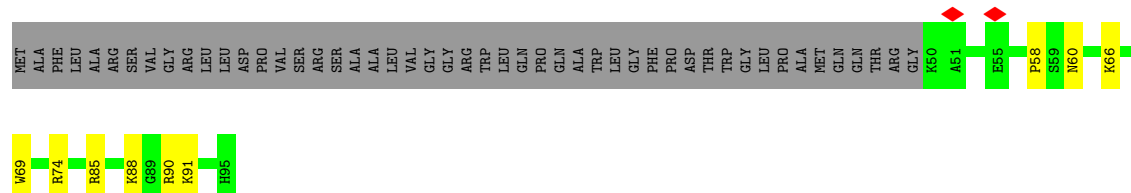
- Molecule 70: Uncharacterized protein

Chain B6: 



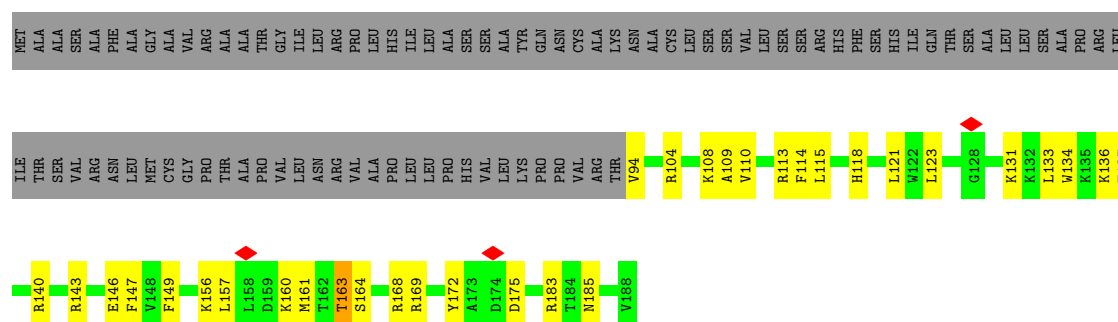
- Molecule 71: Mitochondrial ribosomal protein L34

Chain B7: 



- Molecule 72: Mitochondrial ribosomal protein L35

Chain B8: 



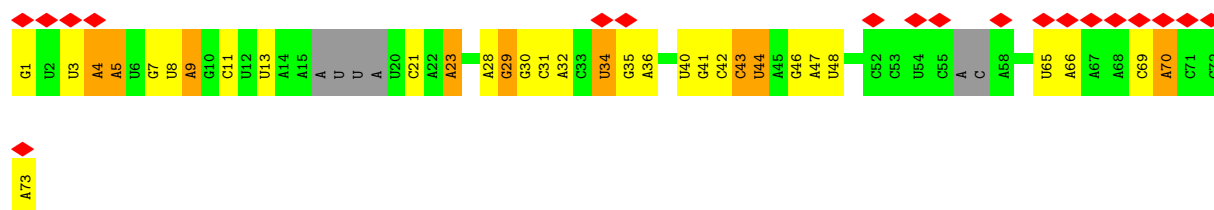
- Molecule 73: Ribosomal protein

Chain B9: 

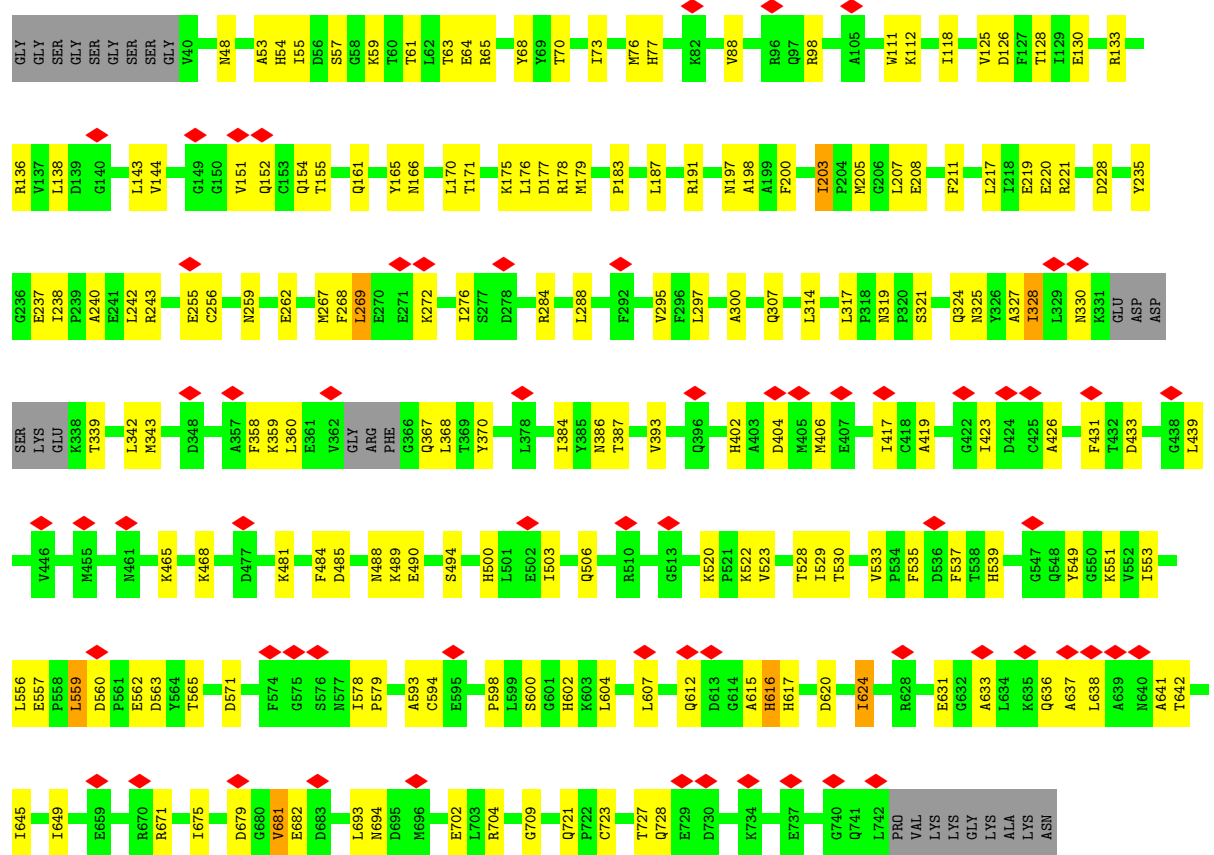
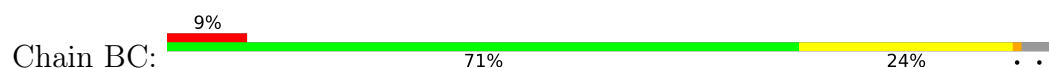




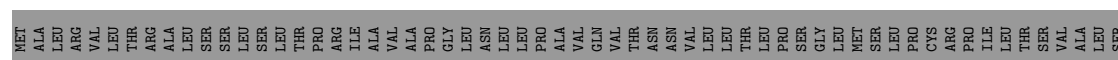
• Molecule 74: CP tRNA-Phe

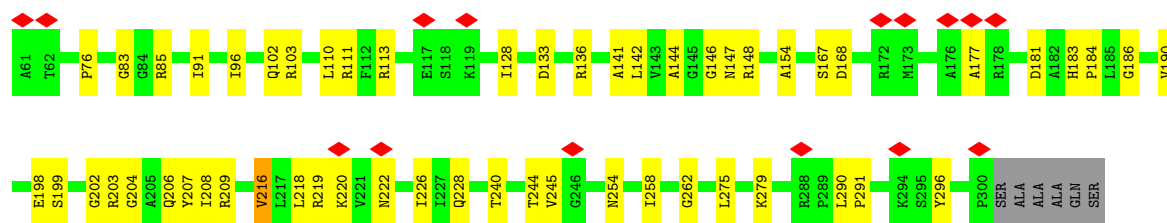


• Molecule 75: Elongation factor G, mitochondrial

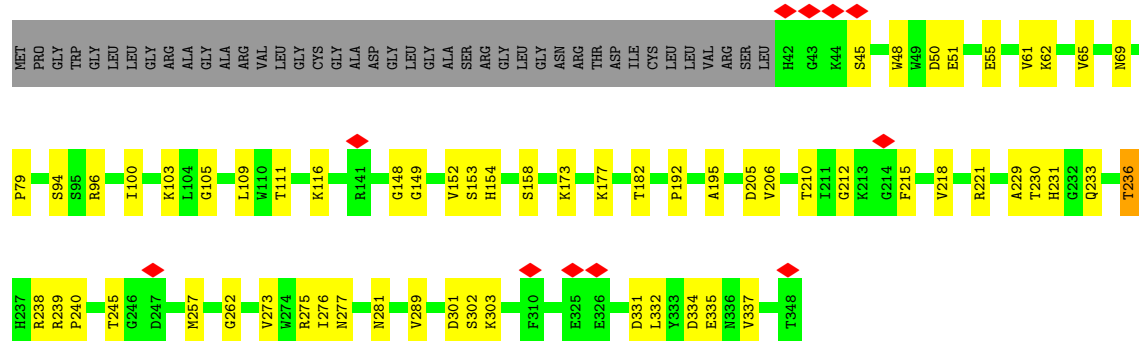


• Molecule 76: Uncharacterized protein

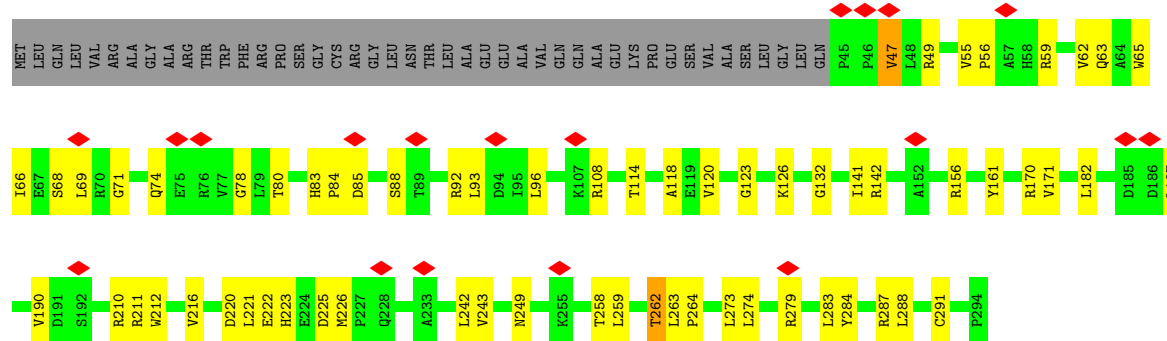




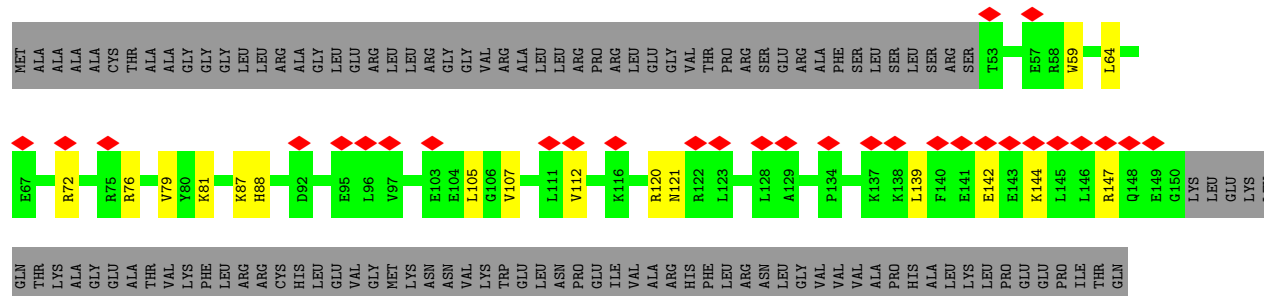
• Molecule 77: ICT1



• Molecule 78: Mitochondrial ribosomal protein L4



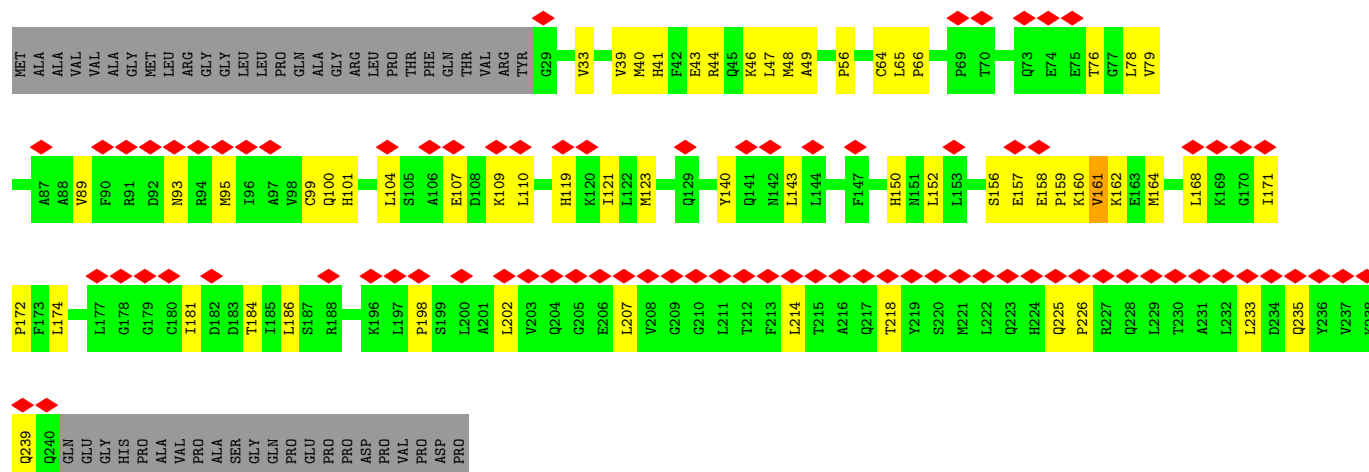
• Molecule 79: Mitochondrial ribosomal protein L9



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

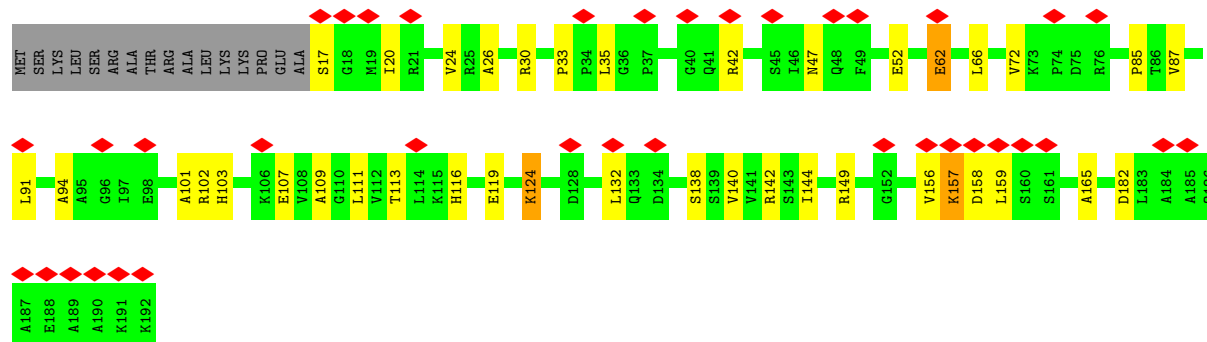
• Molecule 80: Mitochondrial ribosomal protein L10

Chain BJ: 32% 58% 22% 19%



• Molecule 81: Mitochondrial ribosomal protein L11

Chain BK: 19% 71% 19% 8%



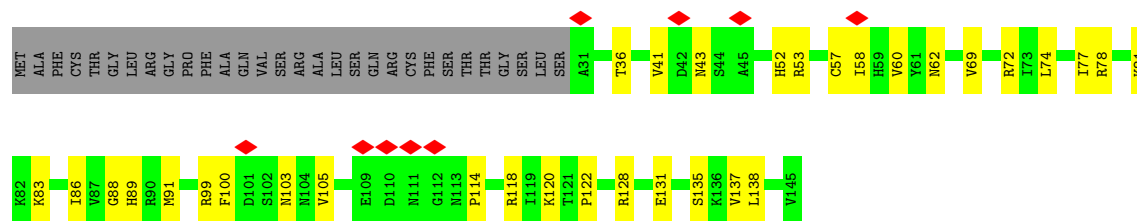
• Molecule 82: Uncharacterized protein

Chain BN: 80% 19%

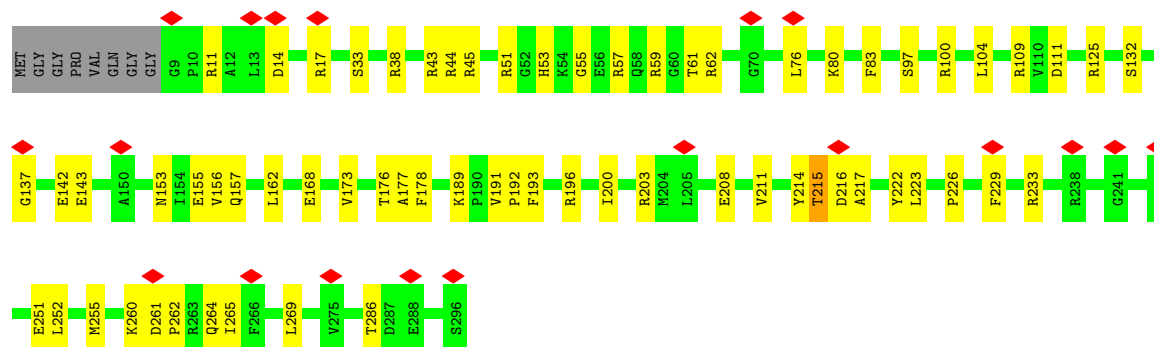
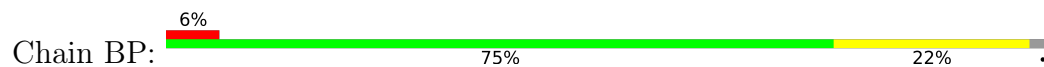


• Molecule 83: Uncharacterized protein

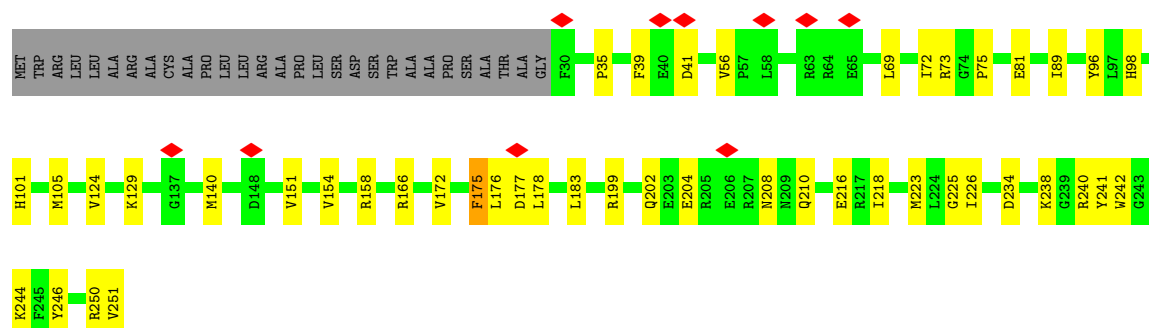
Chain BO: 6% 57% 23% 21%



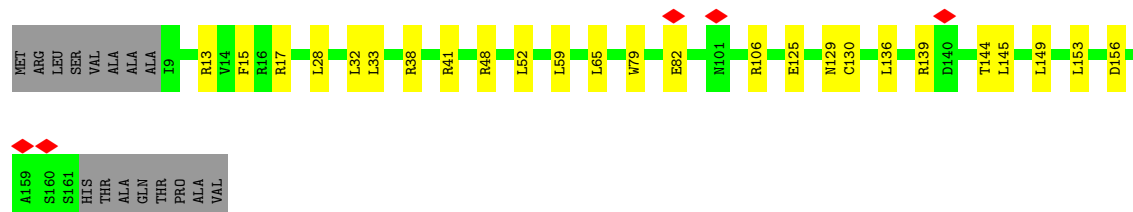
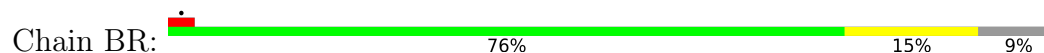
• Molecule 84: Uncharacterized protein



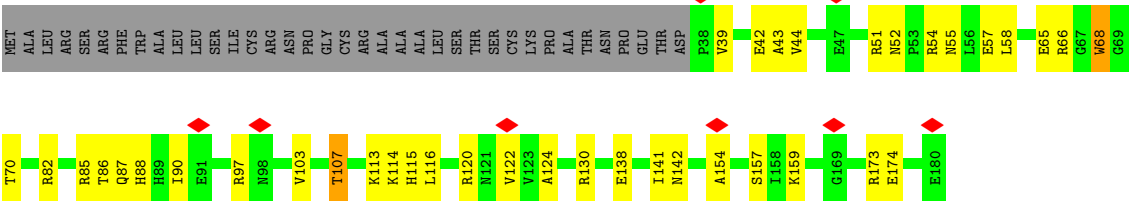
• Molecule 85: Uncharacterized protein



• Molecule 86: Uncharacterized protein



• Molecule 87: Mitochondrial ribosomal protein L18



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, C1                               | Depositor |
| Number of particles used             | 12858                                   | 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 ( $e^-/\text{\AA}^2$ ) | 40                                      | Depositor |
| Minimum defocus (nm)                 | Not provided                            |           |
| Maximum defocus (nm)                 | Not provided                            |           |
| Magnification                        | Not provided                            |           |
| Image detector                       | FEI FALCON III (4k x 4k)                | Depositor |
| Maximum map value                    | 0.289                                   | Depositor |
| Minimum map value                    | -0.162                                  | Depositor |
| Average map value                    | 0.001                                   | Depositor |
| Map value standard deviation         | 0.012                                   | Depositor |
| Recommended contour level            | 0.045                                   | Depositor |
| Map size (Å)                         | 444.8, 444.8, 444.8                     | wwPDB     |
| Map dimensions                       | 320, 320, 320                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.39, 1.39, 1.39                        | 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, GNP, SPM, MG, FME, GTP, 5GP

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   | AI    | 0.10         | 0/2707      | 0.29        | 0/3636        |
| 2   | BT    | 0.09         | 0/1883      | 0.26        | 0/2540        |
| 3   | BU    | 0.11         | 0/1179      | 0.31        | 0/1578        |
| 4   | BV    | 0.11         | 0/1256      | 0.30        | 0/1706        |
| 5   | BW    | 0.11         | 0/1407      | 0.28        | 0/1891        |
| 6   | BX    | 0.12         | 0/1211      | 0.31        | 0/1646        |
| 7   | BY    | 0.10         | 0/1719      | 0.28        | 0/2329        |
| 8   | Ba    | 0.10         | 0/3267      | 0.28        | 0/4455        |
| 9   | Bb    | 0.10         | 0/3047      | 0.29        | 0/4139        |
| 10  | Bc    | 0.09         | 0/2464      | 0.27        | 0/3330        |
| 11  | Bd    | 0.11         | 0/1203      | 0.29        | 0/1622        |
| 12  | Be    | 0.10         | 0/1000      | 0.26        | 0/1345        |
| 13  | Bf    | 0.13         | 0/851       | 0.48        | 2/1159 (0.2%) |
| 14  | Bg    | 0.11         | 0/1191      | 0.31        | 0/1614        |
| 15  | Bh    | 0.10         | 0/2372      | 0.28        | 0/3211        |
| 16  | Bi    | 0.09         | 0/2199      | 0.27        | 0/2980        |
| 17  | Bj    | 0.09         | 0/1811      | 0.27        | 0/2436        |
| 18  | Bk    | 0.10         | 0/1270      | 0.27        | 0/1714        |
| 19  | Bl    | 0.10         | 0/1135      | 0.28        | 0/1549        |
| 20  | Bm    | 0.09         | 0/917       | 0.25        | 0/1248        |
| 21  | Bn    | 0.10         | 0/860       | 0.30        | 0/1150        |
| 22  | Bo    | 0.09         | 0/787       | 0.25        | 0/1056        |
| 23  | Bp    | 0.10         | 0/752       | 0.33        | 0/1013        |
| 24  | Bq    | 0.12         | 0/717       | 0.39        | 1/971 (0.1%)  |
| 25  | Bt    | 0.11         | 0/798       | 0.33        | 0/1073        |
| 26  | Bu    | 0.10         | 0/1214      | 0.36        | 1/1630 (0.1%) |
| 27  | Bv    | 0.10         | 0/1157      | 0.28        | 0/1560        |
| 28  | B0    | 0.10         | 0/880       | 0.25        | 0/1189        |
| 29  | Bw    | 0.10         | 0/3206      | 0.28        | 0/4354        |
| 30  | Bx    | 0.11         | 0/1364      | 0.30        | 0/1849        |
| 31  | AA    | 0.08         | 0/22852     | 0.20        | 0/35580       |
| 31  | BA    | 0.10         | 0/36784     | 0.25        | 0/57270       |

| Mol | Chain | Bond lengths |         | Bond angles |               |
|-----|-------|--------------|---------|-------------|---------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5       |
| 32  | AB    | 0.12         | 0/1804  | 0.33        | 0/2445        |
| 33  | AC    | 0.11         | 0/1105  | 0.33        | 0/1496        |
| 34  | AE    | 0.10         | 0/2785  | 0.29        | 0/3735        |
| 35  | AF    | 0.11         | 0/999   | 0.31        | 0/1347        |
| 36  | AG    | 0.09         | 0/1763  | 0.26        | 0/2368        |
| 37  | AJ    | 0.10         | 0/1181  | 0.29        | 0/1597        |
| 38  | AK    | 0.09         | 0/1027  | 0.28        | 0/1389        |
| 39  | AL    | 0.10         | 0/858   | 0.28        | 0/1152        |
| 40  | AN    | 0.10         | 0/874   | 0.30        | 0/1171        |
| 41  | AO    | 0.10         | 0/1473  | 0.29        | 0/1970        |
| 42  | AP    | 0.11         | 0/954   | 0.32        | 0/1284        |
| 43  | AQ    | 0.10         | 0/894   | 0.26        | 0/1213        |
| 44  | AR    | 0.10         | 0/802   | 0.33        | 0/1079        |
| 45  | AU    | 0.11         | 0/745   | 0.31        | 0/993         |
| 46  | AV    | 0.10         | 0/1673  | 0.25        | 0/2602        |
| 46  | AY    | 0.10         | 0/1673  | 0.27        | 0/2602        |
| 47  | AX    | 0.08         | 0/142   | 0.15        | 0/219         |
| 48  | AZ    | 0.06         | 0/89    | 0.20        | 0/123         |
| 49  | Aa    | 0.10         | 0/2428  | 0.29        | 0/3279        |
| 50  | Ab    | 0.09         | 0/1126  | 0.28        | 0/1514        |
| 51  | Ac    | 0.10         | 0/1399  | 0.28        | 0/1881        |
| 52  | Ad    | 0.12         | 0/1490  | 0.32        | 0/2005        |
| 53  | Ae    | 0.11         | 0/3171  | 0.34        | 1/4292 (0.0%) |
| 54  | B1    | 0.09         | 0/2093  | 0.26        | 0/2835        |
| 55  | Af    | 0.08         | 0/790   | 0.28        | 0/1064        |
| 56  | Ag    | 0.10         | 0/2945  | 0.29        | 0/3984        |
| 57  | Ah    | 0.09         | 0/1045  | 0.26        | 0/1409        |
| 58  | Ai    | 0.10         | 0/841   | 0.33        | 0/1121        |
| 59  | Aj    | 0.11         | 0/1835  | 0.32        | 0/2484        |
| 60  | Ak    | 0.10         | 0/2268  | 0.30        | 0/3069        |
| 61  | Am    | 0.11         | 0/947   | 0.32        | 0/1268        |
| 62  | An    | 0.10         | 0/650   | 0.32        | 0/858         |
| 63  | Ao    | 0.10         | 0/4625  | 0.28        | 0/6267        |
| 64  | Ap    | 0.10         | 0/1616  | 0.27        | 0/2195        |
| 65  | CL    | 0.09         | 0/319   | 0.23        | 0/435         |
| 65  | DL    | 0.08         | 0/212   | 0.25        | 0/286         |
| 65  | EL    | 0.07         | 0/221   | 0.22        | 0/297         |
| 65  | FL    | 0.08         | 0/212   | 0.25        | 0/286         |
| 65  | GL    | 0.08         | 0/212   | 0.22        | 0/286         |
| 65  | HL    | 0.09         | 0/204   | 0.26        | 0/275         |
| 65  | LL    | 0.11         | 0/542   | 0.29        | 0/729         |
| 66  | B2    | 0.09         | 0/1586  | 0.26        | 0/2123        |
| 67  | B3    | 0.10         | 0/993   | 0.27        | 0/1341        |

| Mol | Chain | Bond lengths |          | Bond angles |                 |
|-----|-------|--------------|----------|-------------|-----------------|
|     |       | RMSZ         | # Z  >5  | RMSZ        | # Z  >5         |
| 68  | B4    | 0.12         | 0/481    | 0.40        | 1/653 (0.2%)    |
| 69  | B5    | 0.10         | 0/917    | 0.29        | 0/1227          |
| 70  | B6    | 0.09         | 0/430    | 0.27        | 0/570           |
| 71  | B7    | 0.10         | 0/395    | 0.29        | 0/524           |
| 72  | B8    | 0.10         | 0/853    | 0.29        | 0/1136          |
| 73  | B9    | 0.10         | 0/342    | 0.30        | 0/450           |
| 74  | BB    | 0.08         | 0/1595   | 0.19        | 0/2475          |
| 75  | BC    | 0.11         | 0/5522   | 0.31        | 0/7451          |
| 76  | BD    | 0.10         | 0/1898   | 0.31        | 0/2555          |
| 77  | BE    | 0.09         | 0/2493   | 0.26        | 0/3387          |
| 78  | BF    | 0.10         | 0/2069   | 0.29        | 0/2816          |
| 79  | BI    | 0.10         | 0/819    | 0.28        | 0/1101          |
| 80  | BJ    | 0.10         | 0/1742   | 0.28        | 0/2358          |
| 81  | BK    | 0.10         | 0/1359   | 0.27        | 0/1828          |
| 82  | BN    | 0.10         | 0/1487   | 0.26        | 0/2017          |
| 83  | BO    | 0.11         | 0/912    | 0.30        | 0/1231          |
| 84  | BP    | 0.10         | 0/2368   | 0.30        | 0/3198          |
| 85  | BQ    | 0.10         | 0/1850   | 0.28        | 0/2491          |
| 86  | BR    | 0.11         | 0/1262   | 0.29        | 0/1700          |
| 87  | BS    | 0.11         | 0/1197   | 0.33        | 0/1624          |
| All | All   | 0.10         | 0/190062 | 0.27        | 6/269983 (0.0%) |

There are no bond length outliers.

All (6) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 13  | Bf    | 80  | PRO  | N-CA-CB | 7.51 | 111.14      | 103.25   |
| 53  | Ae    | 342 | PRO  | N-CA-CB | 7.46 | 111.08      | 103.25   |
| 13  | Bf    | 78  | PRO  | N-CA-CB | 7.36 | 110.98      | 103.25   |
| 26  | Bu    | 167 | PRO  | N-CA-CB | 7.35 | 110.97      | 103.25   |
| 24  | Bq    | 59  | PRO  | N-CA-CB | 6.71 | 110.29      | 103.25   |
| 68  | B4    | 87  | PRO  | N-CA-CB | 6.11 | 110.06      | 103.33   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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   | AI    | 2650  | 0        | 2613     | 41      | 0            |
| 2   | BT    | 1840  | 0        | 1855     | 27      | 0            |
| 3   | BU    | 1159  | 0        | 1228     | 26      | 0            |
| 4   | BV    | 1231  | 0        | 1278     | 26      | 0            |
| 5   | BW    | 1374  | 0        | 1405     | 22      | 0            |
| 6   | BX    | 1181  | 0        | 1139     | 21      | 0            |
| 7   | BY    | 1678  | 0        | 1683     | 31      | 0            |
| 8   | Ba    | 3173  | 0        | 3153     | 81      | 0            |
| 9   | Bb    | 2952  | 0        | 2840     | 63      | 0            |
| 10  | Bc    | 2408  | 0        | 2415     | 43      | 0            |
| 11  | Bd    | 1177  | 0        | 1182     | 36      | 0            |
| 12  | Be    | 972   | 0        | 971      | 23      | 0            |
| 13  | Bf    | 827   | 0        | 736      | 14      | 0            |
| 14  | Bg    | 1167  | 0        | 1173     | 22      | 0            |
| 15  | Bh    | 2319  | 0        | 2332     | 43      | 0            |
| 16  | Bi    | 2138  | 0        | 2139     | 41      | 0            |
| 17  | Bj    | 1775  | 0        | 1797     | 46      | 0            |
| 18  | Bk    | 1246  | 0        | 1251     | 22      | 0            |
| 19  | Bl    | 1097  | 0        | 1080     | 14      | 0            |
| 20  | Bm    | 893   | 0        | 878      | 18      | 0            |
| 21  | Bn    | 837   | 0        | 860      | 15      | 0            |
| 22  | Bo    | 772   | 0        | 773      | 15      | 0            |
| 23  | Bp    | 742   | 0        | 749      | 11      | 0            |
| 24  | Bq    | 697   | 0        | 659      | 11      | 0            |
| 25  | Bt    | 780   | 0        | 792      | 24      | 0            |
| 26  | Bu    | 1198  | 0        | 1192     | 16      | 0            |
| 27  | Bv    | 1131  | 0        | 1093     | 12      | 0            |
| 28  | B0    | 857   | 0        | 878      | 15      | 0            |
| 29  | Bw    | 3126  | 0        | 3153     | 57      | 0            |
| 30  | Bx    | 1325  | 0        | 1354     | 29      | 0            |
| 31  | AA    | 20411 | 0        | 10343    | 393     | 0            |
| 31  | BA    | 32844 | 0        | 16617    | 628     | 0            |
| 32  | AB    | 1762  | 0        | 1774     | 27      | 0            |
| 33  | AC    | 1075  | 0        | 1087     | 37      | 0            |
| 34  | AE    | 2732  | 0        | 2774     | 52      | 0            |
| 35  | AF    | 981   | 0        | 1012     | 24      | 0            |
| 36  | AG    | 1721  | 0        | 1747     | 33      | 0            |
| 37  | AJ    | 1155  | 0        | 1193     | 26      | 0            |
| 38  | AK    | 1007  | 0        | 1042     | 18      | 0            |
| 39  | AL    | 840   | 0        | 890      | 17      | 0            |
| 40  | AN    | 858   | 0        | 883      | 21      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 41  | AO    | 1448  | 0        | 1536     | 24      | 0            |
| 42  | AP    | 932   | 0        | 951      | 26      | 0            |
| 43  | AQ    | 875   | 0        | 931      | 19      | 0            |
| 44  | AR    | 784   | 0        | 813      | 14      | 0            |
| 45  | AU    | 734   | 0        | 745      | 16      | 0            |
| 46  | AV    | 1498  | 0        | 765      | 21      | 0            |
| 46  | AY    | 1498  | 0        | 766      | 18      | 0            |
| 47  | AX    | 128   | 0        | 65       | 1       | 0            |
| 48  | AZ    | 90    | 0        | 89       | 2       | 0            |
| 49  | Aa    | 2378  | 0        | 2392     | 42      | 0            |
| 50  | Ab    | 1101  | 0        | 1118     | 11      | 0            |
| 51  | Ac    | 1367  | 0        | 1385     | 18      | 0            |
| 52  | Ad    | 1467  | 0        | 1466     | 24      | 0            |
| 53  | Ae    | 3109  | 0        | 3029     | 53      | 0            |
| 54  | B1    | 2036  | 0        | 2058     | 21      | 0            |
| 55  | Af    | 778   | 0        | 791      | 18      | 0            |
| 56  | Ag    | 2875  | 0        | 2886     | 69      | 0            |
| 57  | Ah    | 1015  | 0        | 969      | 18      | 0            |
| 58  | Ai    | 824   | 0        | 842      | 25      | 0            |
| 59  | Aj    | 1788  | 0        | 1799     | 39      | 0            |
| 60  | Ak    | 2222  | 0        | 2270     | 52      | 0            |
| 61  | Am    | 930   | 0        | 959      | 21      | 0            |
| 62  | An    | 639   | 0        | 709      | 9       | 0            |
| 63  | Ao    | 4525  | 0        | 4433     | 63      | 0            |
| 64  | Ap    | 1564  | 0        | 1531     | 27      | 0            |
| 65  | CL    | 317   | 0        | 309      | 7       | 0            |
| 65  | DL    | 213   | 0        | 234      | 11      | 0            |
| 65  | EL    | 222   | 0        | 247      | 6       | 0            |
| 65  | FL    | 213   | 0        | 234      | 8       | 0            |
| 65  | GL    | 213   | 0        | 234      | 5       | 0            |
| 65  | HL    | 205   | 0        | 223      | 5       | 0            |
| 65  | LL    | 537   | 0        | 591      | 15      | 0            |
| 66  | B2    | 1548  | 0        | 1583     | 19      | 0            |
| 67  | B3    | 968   | 0        | 1018     | 30      | 0            |
| 68  | B4    | 474   | 0        | 454      | 18      | 0            |
| 69  | B5    | 902   | 0        | 916      | 21      | 0            |
| 70  | B6    | 425   | 0        | 471      | 10      | 0            |
| 71  | B7    | 387   | 0        | 413      | 9       | 0            |
| 72  | B8    | 833   | 0        | 883      | 24      | 0            |
| 73  | B9    | 335   | 0        | 359      | 8       | 0            |
| 74  | BB    | 1427  | 0        | 726      | 19      | 0            |
| 75  | BC    | 5425  | 0        | 5412     | 115     | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 76  | BD    | 1860  | 0        | 1922     | 36      | 0            |
| 77  | BE    | 2420  | 0        | 2418     | 46      | 0            |
| 78  | BF    | 2011  | 0        | 2049     | 47      | 0            |
| 79  | BI    | 805   | 0        | 845      | 10      | 0            |
| 80  | BJ    | 1705  | 0        | 1804     | 43      | 0            |
| 81  | BK    | 1339  | 0        | 1407     | 23      | 0            |
| 82  | BN    | 1444  | 0        | 1437     | 34      | 0            |
| 83  | BO    | 896   | 0        | 946      | 26      | 0            |
| 84  | BP    | 2312  | 0        | 2373     | 47      | 0            |
| 85  | BQ    | 1803  | 0        | 1841     | 32      | 0            |
| 86  | BR    | 1240  | 0        | 1260     | 20      | 0            |
| 87  | BS    | 1168  | 0        | 1159     | 35      | 0            |
| 88  | AA    | 102   | 0        | 0        | 0       | 0            |
| 88  | AB    | 1     | 0        | 0        | 0       | 0            |
| 88  | AX    | 1     | 0        | 0        | 0       | 0            |
| 88  | Ag    | 1     | 0        | 0        | 0       | 0            |
| 88  | Am    | 1     | 0        | 0        | 0       | 0            |
| 88  | An    | 1     | 0        | 0        | 0       | 0            |
| 88  | B0    | 1     | 0        | 0        | 0       | 0            |
| 88  | BA    | 200   | 0        | 0        | 0       | 0            |
| 88  | BB    | 1     | 0        | 0        | 0       | 0            |
| 88  | BC    | 2     | 0        | 0        | 0       | 0            |
| 88  | BD    | 3     | 0        | 0        | 0       | 0            |
| 88  | BF    | 1     | 0        | 0        | 0       | 0            |
| 88  | BJ    | 1     | 0        | 0        | 0       | 0            |
| 88  | BP    | 3     | 0        | 0        | 0       | 0            |
| 88  | BQ    | 1     | 0        | 0        | 0       | 0            |
| 88  | BW    | 1     | 0        | 0        | 0       | 0            |
| 88  | Be    | 1     | 0        | 0        | 0       | 0            |
| 88  | Bl    | 1     | 0        | 0        | 0       | 0            |
| 88  | Bq    | 1     | 0        | 0        | 0       | 0            |
| 88  | Bt    | 1     | 0        | 0        | 0       | 0            |
| 89  | AR    | 1     | 0        | 0        | 0       | 0            |
| 89  | Ac    | 1     | 0        | 0        | 0       | 0            |
| 89  | Ap    | 1     | 0        | 0        | 0       | 0            |
| 89  | B5    | 1     | 0        | 0        | 0       | 0            |
| 89  | B9    | 1     | 0        | 0        | 0       | 0            |
| 89  | Bx    | 1     | 0        | 0        | 0       | 0            |
| 90  | AA    | 14    | 0        | 0        | 0       | 0            |
| 90  | BA    | 28    | 0        | 0        | 0       | 0            |
| 91  | AV    | 10    | 0        | 10       | 0       | 0            |
| 92  | Ag    | 32    | 0        | 12       | 0       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 93  | BA    | 24     | 0        | 0        | 0       | 0            |
| 94  | BC    | 32     | 0        | 13       | 3       | 0            |
| 95  | Ag    | 3      | 0        | 0        | 0       | 0            |
| 95  | BC    | 2      | 0        | 0        | 2       | 0            |
| All | All   | 180836 | 0        | 153114   | 2847    | 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 9.

All (2847) 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) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:BA:118:U:H3     | 31:BA:129:A:N6     | 1.44                     | 1.14              |
| 31:AA:405:G:H1     | 31:AA:452:C:HO2'   | 1.17                     | 0.89              |
| 81:BK:113:THR:HG1  | 81:BK:116:HIS:HD1  | 1.24                     | 0.86              |
| 31:BA:56:A:H61     | 31:BA:377:G:H21    | 1.25                     | 0.85              |
| 31:AA:548:G:H1     | 31:AA:785:U:H3     | 1.21                     | 0.84              |
| 15:Bh:97:TYR:HB2   | 15:Bh:181:SER:HA   | 1.63                     | 0.79              |
| 31:AA:11:G:H1      | 31:AA:524:U:H3     | 1.27                     | 0.79              |
| 66:B2:228:LEU:HD11 | 31:BA:11:G:H5'     | 1.65                     | 0.79              |
| 67:B3:74:SER:HB3   | 31:BA:472:U:H5''   | 1.67                     | 0.76              |
| 31:BA:1570:C:H5''  | 31:BA:1571:A:H2'   | 1.66                     | 0.75              |
| 31:BA:392:U:H2'    | 31:BA:393:A:H8     | 1.51                     | 0.75              |
| 31:BA:207:A:H61    | 31:BA:236:U:H3'    | 1.51                     | 0.75              |
| 8:Ba:126:THR:HG22  | 8:Ba:372:ASN:HB2   | 1.68                     | 0.75              |
| 7:BY:161:ARG:HH21  | 7:BY:165:ILE:HB    | 1.52                     | 0.74              |
| 31:BA:118:U:H3     | 31:BA:129:A:H62    | 0.78                     | 0.74              |
| 21:Bn:69:HIS:HD2   | 21:Bn:71:LYS:HG3   | 1.52                     | 0.74              |
| 6:BX:2:ALA:N       | 6:BX:7:TYR:HH      | 1.85                     | 0.74              |
| 63:Ao:485:ILE:HD12 | 63:Ao:491:PRO:HG3  | 1.70                     | 0.74              |
| 31:AA:525:U:H2'    | 31:AA:526:G:H8     | 1.52                     | 0.74              |
| 80:BJ:95:MET:HB2   | 80:BJ:159:PRO:HB3  | 1.69                     | 0.74              |
| 31:BA:1369:U:H5''  | 31:BA:1370:U:H5'   | 1.70                     | 0.74              |
| 31:AA:66:C:H42     | 52:Ad:27:ARG:HB2   | 1.52                     | 0.73              |
| 55:Af:162:THR:HG22 | 55:Af:164:LEU:H    | 1.54                     | 0.73              |
| 31:BA:1291:U:OP2   | 31:BA:1299:C:N4    | 2.21                     | 0.73              |
| 6:BX:41:GLN:NE2    | 31:BA:703:A:OP1    | 2.22                     | 0.73              |
| 8:Ba:160:HIS:HA    | 8:Ba:164:TRP:HB2   | 1.71                     | 0.73              |
| 56:Ag:386:ASN:HD22 | 56:Ag:389:GLN:H    | 1.37                     | 0.72              |
| 35:AF:27:GLU:HG3   | 52:Ad:170:ARG:HH12 | 1.54                     | 0.72              |
| 17:Bj:256:SER:O    | 17:Bj:260:LEU:HB2  | 1.89                     | 0.72              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 63:Ao:460:TYR:HA   | 63:Ao:463:LYS:HE2  | 1.70                     | 0.72              |
| 31:AA:567:C:H2'    | 31:AA:568:G:H8     | 1.53                     | 0.71              |
| 31:BA:602:G:N7     | 84:BP:44:ARG:NH2   | 2.35                     | 0.71              |
| 3:BU:14:VAL:HB     | 3:BU:17:ARG:HH21   | 1.56                     | 0.71              |
| 27:Bv:28:ARG:NH1   | 31:BA:100:C:O2'    | 2.24                     | 0.71              |
| 29:Bw:146:GLN:HA   | 29:Bw:150:PHE:HB2  | 1.73                     | 0.71              |
| 31:BA:831:U:OP2    | 31:BA:836:A:N6     | 2.21                     | 0.71              |
| 65:LL:134:LEU:HD21 | 65:LL:145:LEU:HD21 | 1.72                     | 0.71              |
| 37:AJ:158:GLU:HG2  | 63:Ao:70:ILE:HD13  | 1.72                     | 0.71              |
| 31:AA:492:U:OP1    | 62:An:139:ASN:ND2  | 2.23                     | 0.70              |
| 40:AN:40:ARG:HH12  | 40:AN:86:ARG:HH21  | 1.38                     | 0.70              |
| 63:Ao:543:HIS:HB2  | 63:Ao:588:ARG:HD2  | 1.71                     | 0.70              |
| 66:B2:231:LYS:NZ   | 31:BA:11:G:O6      | 2.25                     | 0.70              |
| 51:Ac:33:ASN:HD21  | 51:Ac:70:MET:HB2   | 1.55                     | 0.70              |
| 31:BA:1459:U:O2    | 31:BA:1468:A:N7    | 2.24                     | 0.70              |
| 31:BA:1330:U:O2    | 31:BA:1406:G:N2    | 2.24                     | 0.70              |
| 31:AA:235:A:H61    | 64:Ap:82:LYS:HG3   | 1.57                     | 0.70              |
| 11:Bd:88:GLU:OE1   | 68:B4:38:ARG:NH1   | 2.24                     | 0.70              |
| 26:Bu:183:ASN:HD22 | 87:BS:142:ASN:HD22 | 1.40                     | 0.70              |
| 31:AA:29:A:H2'     | 31:AA:30:A:H8      | 1.55                     | 0.70              |
| 31:BA:118:U:O4     | 31:BA:129:A:N7     | 2.24                     | 0.70              |
| 30:Bx:108:CYS:HB3  | 80:BJ:64:CYS:SG    | 2.31                     | 0.70              |
| 5:BW:105:GLU:OE1   | 5:BW:116:LYS:NZ    | 2.24                     | 0.69              |
| 19:Bl:110:ILE:HD11 | 19:Bl:157:LEU:HD13 | 1.72                     | 0.69              |
| 31:AA:89:U:H3      | 31:AA:93:A:H61     | 1.40                     | 0.69              |
| 7:BY:146:VAL:HG22  | 7:BY:153:ILE:HG22  | 1.74                     | 0.69              |
| 18:Bk:201:ARG:HD3  | 18:Bk:204:LEU:HD13 | 1.74                     | 0.69              |
| 73:B9:76:CYS:SG    | 73:B9:89:CYS:HB2   | 2.33                     | 0.69              |
| 31:BA:56:A:H61     | 31:BA:377:G:N2     | 1.89                     | 0.69              |
| 21:Bn:77:PRO:HG2   | 21:Bn:80:LEU:HB2   | 1.75                     | 0.69              |
| 31:BA:56:A:N6      | 31:BA:377:G:H21    | 1.90                     | 0.69              |
| 32:AB:93:LYS:HE2   | 55:Af:149:GLU:HB3  | 1.75                     | 0.69              |
| 49:Aa:287:THR:HG23 | 49:Aa:289:HIS:H    | 1.57                     | 0.69              |
| 56:Ag:80:HIS:HB3   | 56:Ag:155:PRO:HG3  | 1.73                     | 0.69              |
| 46:AY:48:G:H2'     | 46:AY:49:G:C8      | 2.28                     | 0.69              |
| 33:AC:69:LEU:HB3   | 33:AC:93:ARG:HH22  | 1.57                     | 0.69              |
| 57:Ah:309:ASN:HD21 | 60:Ak:158:TYR:H    | 1.41                     | 0.68              |
| 56:Ag:230:MET:HG3  | 56:Ag:231:ARG:HG3  | 1.76                     | 0.68              |
| 33:AC:128:PRO:HD2  | 33:AC:131:LYS:HD3  | 1.76                     | 0.68              |
| 14:Bg:73:PRO:HB2   | 14:Bg:89:ILE:HG13  | 1.75                     | 0.68              |
| 31:AA:551:G:N2     | 31:AA:778:G:O2'    | 2.26                     | 0.68              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 33:AC:109:VAL:HB   | 33:AC:120:CYS:HB2  | 1.74                     | 0.68              |
| 75:BC:368:LEU:HD11 | 75:BC:419:ALA:HB1  | 1.74                     | 0.68              |
| 77:BE:221:ARG:NH1  | 77:BE:257:MET:O    | 2.25                     | 0.68              |
| 8:Ba:228:ALA:HB3   | 8:Ba:292:TYR:HB2   | 1.74                     | 0.68              |
| 12:Be:44:ARG:HH12  | 29:Bw:157:ALA:HB3  | 1.57                     | 0.68              |
| 18:Bk:90:VAL:HG12  | 18:Bk:160:SER:HA   | 1.76                     | 0.68              |
| 84:BP:104:LEU:HD22 | 84:BP:109:ARG:HD2  | 1.76                     | 0.68              |
| 31:AA:194:U:H2'    | 31:AA:195:G:H8     | 1.59                     | 0.68              |
| 16:Bi:42:THR:HG21  | 78:BF:132:GLY:HA3  | 1.74                     | 0.68              |
| 82:BN:27:PRO:HG2   | 82:BN:30:LYS:HB2   | 1.76                     | 0.68              |
| 32:AB:137:ARG:HD3  | 50:Ab:34:ILE:HD11  | 1.74                     | 0.68              |
| 38:AK:68:ILE:HG12  | 38:AK:70:GLY:H     | 1.58                     | 0.68              |
| 31:BA:1230:U:H5'   | 31:BA:1231:U:H5'   | 1.76                     | 0.68              |
| 49:Aa:184:SER:H    | 49:Aa:192:ARG:HH12 | 1.40                     | 0.67              |
| 31:BA:148:A:H4'    | 31:BA:149:A:H5''   | 1.76                     | 0.67              |
| 25:Bt:23:ARG:NH1   | 31:BA:464:U:OP1    | 2.27                     | 0.67              |
| 31:BA:222:G:N7     | 78:BF:170:ARG:NH2  | 2.39                     | 0.67              |
| 31:BA:524:C:O2'    | 81:BK:149:ARG:NH2  | 2.27                     | 0.67              |
| 8:Ba:236:LEU:HB3   | 8:Ba:341:VAL:HG13  | 1.77                     | 0.67              |
| 71:B7:85:ARG:HE    | 71:B7:90:ARG:HG3   | 1.59                     | 0.67              |
| 31:BA:53:U:O4      | 31:BA:62:C:N3      | 2.28                     | 0.67              |
| 2:BT:122:ALA:HB2   | 2:BT:172:GLN:HE21  | 1.60                     | 0.67              |
| 4:BV:88:ASN:ND2    | 4:BV:206:PRO:O     | 2.28                     | 0.67              |
| 14:Bg:28:ARG:HG2   | 14:Bg:78:GLU:HB2   | 1.76                     | 0.67              |
| 31:AA:84:A:N6      | 31:AA:98:A:O2'     | 2.27                     | 0.67              |
| 77:BE:277:ASN:ND2  | 77:BE:331:ASP:OD1  | 2.27                     | 0.67              |
| 31:BA:869:G:O2'    | 31:BA:966:U:OP2    | 2.13                     | 0.67              |
| 14:Bg:133:PHE:HZ   | 15:Bh:261:SER:HB2  | 1.60                     | 0.67              |
| 51:Ac:88:VAL:HG22  | 52:Ad:109:ASN:HD21 | 1.59                     | 0.67              |
| 72:B8:108:LYS:NZ   | 31:BA:77:U:OP2     | 2.28                     | 0.67              |
| 8:Ba:280:GLN:HG2   | 29:Bw:152:ARG:HE   | 1.60                     | 0.67              |
| 31:AA:689:G:HO2'   | 58:Ai:75:HIS:HE2   | 1.43                     | 0.66              |
| 35:AF:15:ARG:NH2   | 52:Ad:182:ASP:OD1  | 2.29                     | 0.66              |
| 59:Aj:132:GLU:HG2  | 59:Aj:133:GLN:HG3  | 1.77                     | 0.66              |
| 31:BA:789:A:N6     | 31:BA:1000:A:O2'   | 2.27                     | 0.66              |
| 18:Bk:124:SER:O    | 74:BB:35:G:N2      | 2.28                     | 0.66              |
| 31:AA:590:C:H2'    | 31:AA:591:A:H8     | 1.59                     | 0.66              |
| 31:BA:470:C:HO2'   | 31:BA:485:A:HO2'   | 1.43                     | 0.66              |
| 27:Bv:63:ARG:NH2   | 31:BA:95:U:OP1     | 2.28                     | 0.66              |
| 56:Ag:124:VAL:HG22 | 56:Ag:307:LEU:HB2  | 1.77                     | 0.66              |
| 9:Bb:221:LEU:HB2   | 9:Bb:267:ARG:HG3   | 1.78                     | 0.66              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 53:Ae:167:TYR:O    | 53:Ae:171:ASN:ND2  | 2.29                     | 0.66              |
| 17:Bj:264:LEU:HD13 | 17:Bj:269:LEU:HB3  | 1.78                     | 0.66              |
| 31:AA:227:A:H61    | 31:AA:270:C:H42    | 1.42                     | 0.66              |
| 31:BA:877:U:H5'    | 31:BA:878:G:H5'    | 1.76                     | 0.66              |
| 31:AA:957:A:OP2    | 61:Am:24:ASN:ND2   | 2.27                     | 0.66              |
| 31:BA:198:U:H2'    | 31:BA:199:A:H8     | 1.61                     | 0.66              |
| 31:BA:1158:C:O2'   | 31:BA:1251:C:OP2   | 2.14                     | 0.66              |
| 21:Bn:35:ARG:NH1   | 21:Bn:37:THR:O     | 2.29                     | 0.66              |
| 3:BU:55:ARG:NH1    | 31:BA:177:U:O2'    | 2.29                     | 0.65              |
| 9:Bb:371:ASP:OD1   | 72:B8:185:ASN:ND2  | 2.30                     | 0.65              |
| 72:B8:157:LEU:HG   | 72:B8:161:MET:HE2  | 1.78                     | 0.65              |
| 73:B9:69:LEU:H     | 31:BA:560:A:H62    | 1.44                     | 0.65              |
| 77:BE:206:VAL:HG11 | 77:BE:289:VAL:HG13 | 1.76                     | 0.65              |
| 35:AF:15:ARG:NH2   | 52:Ad:178:GLU:OE1  | 2.27                     | 0.65              |
| 31:BA:1046:A:OP1   | 77:BE:239:ARG:NH1  | 2.29                     | 0.65              |
| 77:BE:236:THR:HG23 | 77:BE:239:ARG:HD2  | 1.79                     | 0.65              |
| 29:Bw:240:GLN:OE1  | 29:Bw:347:ARG:NH1  | 2.29                     | 0.65              |
| 31:AA:868:U:H3     | 31:AA:902:C:H42    | 1.45                     | 0.65              |
| 34:AE:150:ARG:HG2  | 34:AE:155:GLN:HG2  | 1.78                     | 0.65              |
| 37:AJ:176:LYS:HB3  | 60:Ak:153:ILE:HB   | 1.79                     | 0.65              |
| 50:Ab:71:ARG:HH12  | 55:Af:91:THR:HG22  | 1.60                     | 0.65              |
| 14:Bg:17:ASN:HD21  | 14:Bg:23:VAL:H     | 1.41                     | 0.65              |
| 28:B0:71:ARG:NH2   | 31:BA:1163:A:OP1   | 2.30                     | 0.65              |
| 46:AV:48:G:H2'     | 46:AV:49:G:C8      | 2.32                     | 0.65              |
| 76:BD:110:LEU:HD23 | 76:BD:113:ARG:HE   | 1.61                     | 0.65              |
| 31:AA:272:A:H4'    | 31:AA:274:A:H4'    | 1.77                     | 0.65              |
| 31:BA:225:C:OP1    | 84:BP:132:SER:OG   | 2.14                     | 0.65              |
| 80:BJ:198:PRO:HB3  | 80:BJ:202:LEU:HD23 | 1.78                     | 0.65              |
| 84:BP:142:GLU:HG3  | 84:BP:162:LEU:HD23 | 1.78                     | 0.65              |
| 32:AB:219:VAL:HG22 | 32:AB:233:TYR:HB2  | 1.78                     | 0.65              |
| 60:Ak:154:ASP:HB2  | 60:Ak:174:THR:HB   | 1.78                     | 0.65              |
| 31:BA:446:C:H2'    | 31:BA:447:A:C8     | 2.32                     | 0.65              |
| 4:BV:119:LEU:HD11  | 4:BV:194:GLN:HB3   | 1.79                     | 0.65              |
| 31:AA:50:U:H2'     | 31:AA:51:G:H8      | 1.62                     | 0.65              |
| 31:AA:64:C:OP1     | 42:AP:13:ARG:NH2   | 2.30                     | 0.65              |
| 38:AK:190:PRO:HG2  | 45:AU:45:TYR:HB2   | 1.79                     | 0.65              |
| 56:Ag:358:TYR:O    | 56:Ag:362:ASN:ND2  | 2.30                     | 0.65              |
| 59:Aj:36:LEU:HD11  | 59:Aj:50:LEU:HD11  | 1.79                     | 0.65              |
| 9:Bb:27:ARG:N      | 31:BA:1168:A:N1    | 2.45                     | 0.65              |
| 60:Ak:178:LYS:HE2  | 60:Ak:180:SER:HB3  | 1.78                     | 0.65              |
| 67:B3:69:VAL:HG12  | 67:B3:119:ILE:HG12 | 1.79                     | 0.65              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:BA:129:A:OP1    | 78:BF:142:ARG:NH2  | 2.30                     | 0.65              |
| 31:BA:1309:U:H2'   | 31:BA:1310:A:H8    | 1.62                     | 0.65              |
| 83:BO:58:ILE:HG21  | 83:BO:74:LEU:HD23  | 1.78                     | 0.65              |
| 18:Bk:48:TYR:N     | 31:BA:402:A:OP1    | 2.30                     | 0.64              |
| 31:AA:587:U:O2     | 31:AA:707:A:N6     | 2.30                     | 0.64              |
| 56:Ag:185:THR:O    | 56:Ag:189:ASN:ND2  | 2.29                     | 0.64              |
| 77:BE:50:ASP:O     | 86:BR:139:ARG:NH1  | 2.30                     | 0.64              |
| 7:BY:191:LEU:HG    | 12:Be:93:THR:HG21  | 1.78                     | 0.64              |
| 31:AA:468:A:OP2    | 32:AB:99:ARG:NH2   | 2.31                     | 0.64              |
| 66:B2:200:ARG:O    | 31:BA:31:A:N6      | 2.27                     | 0.64              |
| 31:AA:647:A:N6     | 45:AU:80:ARG:O     | 2.31                     | 0.64              |
| 80:BJ:47:LEU:HD22  | 85:BQ:226:ILE:HG12 | 1.78                     | 0.64              |
| 87:BS:122:VAL:HG13 | 87:BS:157:SER:HA   | 1.79                     | 0.64              |
| 31:AA:328:A:H2'    | 31:AA:329:A:H8     | 1.63                     | 0.64              |
| 75:BC:637:ALA:O    | 75:BC:641:ALA:HB2  | 1.98                     | 0.64              |
| 1:AI:366:ARG:HB3   | 1:AI:371:LEU:HD12  | 1.78                     | 0.64              |
| 42:AP:53:SER:H     | 42:AP:67:ALA:HB3   | 1.61                     | 0.64              |
| 31:BA:234:G:N2     | 84:BP:33:SER:O     | 2.29                     | 0.64              |
| 84:BP:137:GLY:HA3  | 84:BP:157:GLN:HG3  | 1.80                     | 0.64              |
| 8:Ba:377:ASP:OD1   | 8:Ba:380:GLN:NE2   | 2.30                     | 0.64              |
| 33:AC:163:VAL:HG11 | 33:AC:167:ILE:HB   | 1.79                     | 0.64              |
| 31:BA:243:A:N3     | 31:BA:1266:U:O2'   | 2.30                     | 0.64              |
| 75:BC:219:GLU:OE1  | 75:BC:221:ARG:NH2  | 2.30                     | 0.64              |
| 8:Ba:144:ARG:O     | 8:Ba:194:LYS:NZ    | 2.29                     | 0.64              |
| 18:Bk:147:ASP:OD1  | 68:B4:73:ARG:NH1   | 2.30                     | 0.64              |
| 31:BA:112:A:N6     | 31:BA:115:U:OP2    | 2.30                     | 0.64              |
| 31:BA:1140:A:H2'   | 31:BA:1141:A:H8    | 1.63                     | 0.64              |
| 46:AV:60:C:H2'     | 46:AV:61:C:C6      | 2.33                     | 0.64              |
| 57:Ah:326:LEU:HB2  | 57:Ah:347:THR:HG23 | 1.80                     | 0.64              |
| 31:BA:614:U:O4     | 31:BA:620:A:N6     | 2.31                     | 0.64              |
| 10:Bc:303:ARG:NH2  | 77:BE:45:SER:O     | 2.30                     | 0.63              |
| 52:Ad:168:ILE:HG12 | 52:Ad:176:ARG:HG3  | 1.80                     | 0.63              |
| 56:Ag:267:LEU:O    | 56:Ag:293:ARG:NH2  | 2.31                     | 0.63              |
| 31:BA:197:U:H2'    | 31:BA:198:U:H6     | 1.63                     | 0.63              |
| 31:BA:187:G:H1'    | 31:BA:467:A:N6     | 2.14                     | 0.63              |
| 3:BU:85:ALA:O      | 3:BU:89:ASN:ND2    | 2.32                     | 0.63              |
| 6:BX:37:GLU:HB3    | 6:BX:104:THR:HG23  | 1.79                     | 0.63              |
| 1:AI:251:ILE:HG23  | 1:AI:253:SER:H     | 1.63                     | 0.63              |
| 10:Bc:278:SER:O    | 10:Bc:317:ARG:NH1  | 2.31                     | 0.63              |
| 65:GL:79:ILE:HG23  | 80:BJ:233:LEU:HG   | 1.81                     | 0.63              |
| 31:BA:135:G:N1     | 31:BA:138:A:OP2    | 2.28                     | 0.63              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 75:BC:330:ASN:ND2  | 75:BC:339:THR:OG1 | 2.32                     | 0.63              |
| 85:BQ:202:GLN:NE2  | 85:BQ:251:VAL:O   | 2.31                     | 0.63              |
| 46:AV:9:C:O2'      | 46:AV:10:A:N7     | 2.32                     | 0.63              |
| 31:BA:165:A:H2'    | 31:BA:166:A:H8    | 1.64                     | 0.63              |
| 3:BU:146:VAL:HG11  | 13:Bf:56:ARG:HG2  | 1.81                     | 0.63              |
| 25:Bt:66:ARG:NH2   | 31:BA:417:G:OP1   | 2.30                     | 0.63              |
| 31:BA:1034:G:OP1   | 82:BN:114:LYS:NZ  | 2.29                     | 0.63              |
| 27:Bv:103:LEU:HD21 | 84:BP:208:GLU:HB3 | 1.81                     | 0.63              |
| 30:Bx:152:THR:HA   | 82:BN:69:GLY:HA2  | 1.80                     | 0.63              |
| 63:Ao:586:PHE:HD1  | 63:Ao:591:ARG:HB3 | 1.62                     | 0.63              |
| 30:Bx:164:ASN:O    | 31:BA:568:C:O2'   | 2.15                     | 0.63              |
| 31:AA:677:C:O2     | 34:AE:234:LYS:NZ  | 2.32                     | 0.63              |
| 41:AO:110:MET:SD   | 41:AO:114:ASN:ND2 | 2.72                     | 0.63              |
| 17:Bj:265:LYS:HG3  | 17:Bj:266:PRO:HD3 | 1.80                     | 0.63              |
| 67:B3:72:ILE:HD11  | 67:B3:118:ARG:HB2 | 1.81                     | 0.63              |
| 31:BA:528:U:O4     | 80:BJ:109:LYS:NZ  | 2.31                     | 0.63              |
| 69:B5:181:ARG:NH1  | 69:B5:187:GLN:OE1 | 2.32                     | 0.62              |
| 9:Bb:194:THR:OG1   | 9:Bb:197:GLU:OE1  | 2.17                     | 0.62              |
| 29:Bw:264:LYS:NZ   | 31:BA:705:U:O4    | 2.28                     | 0.62              |
| 31:BA:1081:U:O4    | 31:BA:1135:C:N3   | 2.32                     | 0.62              |
| 31:BA:1569:A:N6    | 77:BE:152:VAL:O   | 2.32                     | 0.62              |
| 31:AA:590:C:H2'    | 31:AA:591:A:C8    | 2.34                     | 0.62              |
| 34:AE:215:TYR:HH   | 50:Ab:2:ALA:N     | 1.96                     | 0.62              |
| 31:BA:118:U:N3     | 31:BA:129:A:N6    | 2.24                     | 0.62              |
| 5:BW:131:ASN:O     | 16:Bi:230:ARG:NH2 | 2.32                     | 0.62              |
| 30:Bx:176:VAL:HG22 | 82:BN:69:GLY:HA3  | 1.80                     | 0.62              |
| 87:BS:116:LEU:HD21 | 87:BS:124:ALA:HA  | 1.80                     | 0.62              |
| 29:Bw:82:ILE:O     | 31:BA:777:A:N6    | 2.29                     | 0.62              |
| 62:An:177:TRP:HB2  | 62:An:182:LEU:HB2 | 1.80                     | 0.62              |
| 25:Bt:41:THR:O     | 25:Bt:45:ASN:ND2  | 2.32                     | 0.62              |
| 43:AQ:95:VAL:HG23  | 43:AQ:96:THR:HG23 | 1.80                     | 0.62              |
| 46:AY:24:U:H2'     | 46:AY:25:C:H6     | 1.64                     | 0.62              |
| 53:Ae:294:GLY:O    | 53:Ae:298:ARG:NH1 | 2.32                     | 0.62              |
| 56:Ag:259:VAL:HG23 | 56:Ag:305:ILE:HA  | 1.82                     | 0.62              |
| 65:DL:84:GLU:HG3   | 65:DL:87:LYS:HE2  | 1.80                     | 0.62              |
| 31:BA:571:A:H2     | 82:BN:111:MET:HE3 | 1.65                     | 0.62              |
| 2:BT:148:THR:HG22  | 2:BT:165:GLU:HG2  | 1.82                     | 0.62              |
| 31:AA:689:G:O2'    | 58:Ai:75:HIS:NE2  | 2.27                     | 0.62              |
| 31:AA:882:A:O2'    | 53:Ae:140:ASN:ND2 | 2.32                     | 0.62              |
| 46:AY:25:C:H2'     | 46:AY:26:G:H8     | 1.65                     | 0.62              |
| 31:BA:238:C:O2'    | 84:BP:51:ARG:NH2  | 2.31                     | 0.62              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:Bo:78:VAL:HG21  | 67:B3:134:MET:HE1  | 1.82                     | 0.62              |
| 10:Bc:112:MET:HB2  | 10:Bc:267:PRO:HB3  | 1.82                     | 0.62              |
| 31:AA:441:U:H2'    | 31:AA:442:A:H8     | 1.64                     | 0.62              |
| 31:AA:630:A:H1'    | 31:AA:655:G:H22    | 1.65                     | 0.62              |
| 49:Aa:344:ALA:HB1  | 49:Aa:348:HIS:HB3  | 1.79                     | 0.62              |
| 31:BA:376:A:N6     | 31:BA:1061:U:O2    | 2.33                     | 0.62              |
| 31:BA:891:A:H3'    | 31:BA:892:G:H8     | 1.65                     | 0.62              |
| 6:BX:143:GLY:O     | 16:Bi:179:LYS:NZ   | 2.33                     | 0.62              |
| 11:Bd:53:LYS:NZ    | 17:Bj:86:ASP:OD1   | 2.32                     | 0.62              |
| 34:AE:392:ARG:HG2  | 34:AE:394:ASP:H    | 1.65                     | 0.62              |
| 41:AO:116:VAL:O    | 41:AO:181:LYS:NZ   | 2.33                     | 0.62              |
| 17:Bj:162:ARG:HB3  | 17:Bj:251:HIS:HB2  | 1.82                     | 0.61              |
| 18:Bk:120:LYS:NZ   | 18:Bk:122:GLU:OE1  | 2.31                     | 0.61              |
| 32:AB:71:PHE:O     | 32:AB:262:LYS:NZ   | 2.33                     | 0.61              |
| 78:BF:223:HIS:HA   | 78:BF:226:MET:HE3  | 1.81                     | 0.61              |
| 2:BT:158:GLN:HE21  | 83:BO:100:PHE:HB3  | 1.64                     | 0.61              |
| 31:BA:233:A:H2'    | 31:BA:234:G:H8     | 1.65                     | 0.61              |
| 13:Bf:127:GLY:N    | 31:BA:159:A:OP2    | 2.34                     | 0.61              |
| 31:AA:185:A:H1'    | 31:AA:213:G:H22    | 1.64                     | 0.61              |
| 42:AP:20:ARG:NH2   | 42:AP:41:CYS:SG    | 2.73                     | 0.61              |
| 49:Aa:198:GLU:OE2  | 49:Aa:204:ARG:NH1  | 2.33                     | 0.61              |
| 53:Ae:204:VAL:HG13 | 53:Ae:221:LEU:HD13 | 1.81                     | 0.61              |
| 10:Bc:282:ASN:HD21 | 10:Bc:289:LEU:HD12 | 1.66                     | 0.61              |
| 46:AV:4:A:H2'      | 46:AV:5:A:C8       | 2.35                     | 0.61              |
| 78:BF:283:LEU:HB2  | 84:BP:125:ARG:HH12 | 1.66                     | 0.61              |
| 85:BQ:39:PHE:O     | 85:BQ:166:ARG:NH1  | 2.34                     | 0.61              |
| 19:Bl:138:THR:HG22 | 19:Bl:149:VAL:HG12 | 1.81                     | 0.61              |
| 29:Bw:53:ALA:O     | 29:Bw:62:ARG:NH2   | 2.27                     | 0.61              |
| 37:AJ:78:VAL:HB    | 37:AJ:143:LEU:HB2  | 1.81                     | 0.61              |
| 50:Ab:89:ASN:HB3   | 50:Ab:92:PHE:HB2   | 1.81                     | 0.61              |
| 68:B4:43:ARG:NH2   | 74:BB:32:A:OP1     | 2.33                     | 0.61              |
| 72:B8:172:TYR:HB2  | 72:B8:175:ASP:HB2  | 1.83                     | 0.61              |
| 75:BC:617:HIS:HD2  | 75:BC:620:ASP:H    | 1.47                     | 0.61              |
| 15:Bh:96:CYS:SG    | 15:Bh:181:SER:OG   | 2.57                     | 0.61              |
| 39:AL:61:VAL:HG12  | 39:AL:107:VAL:HG22 | 1.81                     | 0.61              |
| 66:B2:172:ARG:NH1  | 31:BA:22:U:O4      | 2.34                     | 0.61              |
| 71:B7:58:PRO:HB2   | 31:BA:672:G:H4'    | 1.81                     | 0.61              |
| 75:BC:152:GLN:O    | 75:BC:155:THR:N    | 2.31                     | 0.61              |
| 81:BK:138:SER:OG   | 81:BK:142:ARG:NH1  | 2.33                     | 0.61              |
| 19:Bl:84:TYR:OH    | 19:Bl:164:LYS:NZ   | 2.33                     | 0.61              |
| 33:AC:37:ASN:O     | 33:AC:43:ARG:NH2   | 2.34                     | 0.61              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 56:Ag:173:ASN:O    | 56:Ag:176:ARG:NH1  | 2.34                     | 0.61              |
| 31:BA:569:C:N4     | 31:BA:1020:C:O2    | 2.33                     | 0.61              |
| 31:AA:58:U:OP1     | 59:Aj:53:ARG:NH1   | 2.34                     | 0.61              |
| 42:AP:111:ARG:NH2  | 49:Aa:168:LYS:O    | 2.33                     | 0.61              |
| 73:B9:82:ARG:NH1   | 31:BA:1512:U:OP2   | 2.34                     | 0.61              |
| 25:Bt:78:GLN:NE2   | 31:BA:420:U:O4     | 2.34                     | 0.61              |
| 31:AA:962:C:O2'    | 61:Am:37:ARG:NH2   | 2.34                     | 0.61              |
| 2:BT:183:LEU:HD21  | 2:BT:219:GLN:HG2   | 1.83                     | 0.61              |
| 10:Bc:315:ARG:HD2  | 86:BR:153:LEU:HG   | 1.83                     | 0.61              |
| 37:AJ:179:GLN:HA   | 60:Ak:149:PHE:HA   | 1.82                     | 0.61              |
| 56:Ag:79:PRO:HG2   | 56:Ag:193:ALA:HA   | 1.83                     | 0.61              |
| 65:LL:143:VAL:HG13 | 75:BC:269:LEU:HD13 | 1.81                     | 0.61              |
| 31:BA:993:U:OP2    | 77:BE:238:ARG:NH2  | 2.34                     | 0.61              |
| 31:BA:1354:A:H61   | 31:BA:1465:A:H61   | 1.48                     | 0.61              |
| 8:Ba:30:ALA:N      | 76:BD:202:GLY:O    | 2.34                     | 0.60              |
| 18:Bk:185:SER:HB3  | 18:Bk:187:ARG:HE   | 1.65                     | 0.60              |
| 26:Bu:101:ARG:HG2  | 26:Bu:133:ILE:HG12 | 1.83                     | 0.60              |
| 29:Bw:251:ILE:HG22 | 29:Bw:253:ILE:H    | 1.64                     | 0.60              |
| 49:Aa:205:LYS:NZ   | 64:Ap:182:GLY:O    | 2.33                     | 0.60              |
| 60:Ak:76:ALA:O     | 60:Ak:112:ASN:ND2  | 2.31                     | 0.60              |
| 77:BE:210:THR:OG1  | 77:BE:262:GLY:O    | 2.19                     | 0.60              |
| 35:AF:3:ARG:NH2    | 41:AO:100:ASN:OD1  | 2.33                     | 0.60              |
| 60:Ak:176:ARG:HG2  | 60:Ak:208:THR:HG22 | 1.81                     | 0.60              |
| 1:AI:221:GLN:NE2   | 31:AA:647:A:OP2    | 2.35                     | 0.60              |
| 16:Bi:161:HIS:O    | 16:Bi:260:ARG:NH2  | 2.34                     | 0.60              |
| 29:Bw:85:LYS:HE2   | 31:BA:777:A:H62    | 1.66                     | 0.60              |
| 31:AA:525:U:H2'    | 31:AA:526:G:C8     | 2.36                     | 0.60              |
| 31:BA:881:C:H4'    | 31:BA:882:A:H5'    | 1.83                     | 0.60              |
| 7:BY:52:GLU:O      | 7:BY:143:ARG:NH2   | 2.34                     | 0.60              |
| 10:Bc:230:ASN:HB3  | 10:Bc:233:LYS:HB2  | 1.83                     | 0.60              |
| 31:AA:355:U:H2'    | 31:AA:356:A:H8     | 1.66                     | 0.60              |
| 31:BA:248:A:OP1    | 31:BA:323:A:N6     | 2.32                     | 0.60              |
| 31:BA:801:G:H4'    | 83:BO:36:THR:HG22  | 1.84                     | 0.60              |
| 31:BA:1405:A:H2'   | 31:BA:1406:G:C8    | 2.37                     | 0.60              |
| 9:Bb:279:ILE:HD11  | 9:Bb:310:ALA:HB3   | 1.83                     | 0.60              |
| 31:AA:586:U:OP1    | 40:AN:36:ARG:NH2   | 2.34                     | 0.60              |
| 41:AO:96:LEU:HD11  | 41:AO:107:ILE:HG13 | 1.82                     | 0.60              |
| 54:B1:96:LYS:O     | 31:BA:60:U:O2'     | 2.19                     | 0.60              |
| 67:B3:78:ARG:O     | 67:B3:83:LYS:NZ    | 2.33                     | 0.60              |
| 11:Bd:57:ARG:HD2   | 11:Bd:58:PRO:HD2   | 1.83                     | 0.60              |
| 31:AA:584:C:O2     | 40:AN:86:ARG:NH1   | 2.35                     | 0.60              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 86:BR:38:ARG:NH1   | 86:BR:82:GLU:OE1   | 2.34                     | 0.60              |
| 8:Ba:123:LEU:HD22  | 8:Ba:220:LEU:HD11  | 1.82                     | 0.60              |
| 56:Ag:137:LEU:HD11 | 56:Ag:260:ALA:HB1  | 1.81                     | 0.60              |
| 31:BA:1385:U:H3    | 31:BA:1389:A:H62   | 1.48                     | 0.60              |
| 75:BC:98:ARG:HH22  | 75:BC:506:GLN:HE22 | 1.49                     | 0.60              |
| 75:BC:723:CYS:SG   | 75:BC:727:THR:OG1  | 2.54                     | 0.60              |
| 7:BY:112:GLU:OE1   | 16:Bi:74:ARG:NH1   | 2.35                     | 0.60              |
| 9:Bb:139:TRP:CD1   | 9:Bb:143:CYS:HG    | 2.20                     | 0.60              |
| 29:Bw:63:VAL:HA    | 29:Bw:66:TRP:CD1   | 2.35                     | 0.60              |
| 31:AA:620:C:H2'    | 31:AA:621:A:H8     | 1.65                     | 0.60              |
| 31:AA:850:U:H5'    | 62:An:142:LYS:HZ1  | 1.66                     | 0.60              |
| 69:B5:134:THR:OG1  | 86:BR:41:ARG:NH2   | 2.35                     | 0.60              |
| 72:B8:131:LYS:NZ   | 31:BA:1234:U:OP2   | 2.35                     | 0.60              |
| 8:Ba:162:ARG:NH1   | 8:Ba:383:TYR:OH    | 2.35                     | 0.60              |
| 31:AA:471:U:OP2    | 50:Ab:50:ARG:NH2   | 2.35                     | 0.60              |
| 36:AG:78:PRO:HG2   | 36:AG:81:LYS:HB3   | 1.83                     | 0.60              |
| 65:CL:63:LYS:HD3   | 65:DL:74:LEU:HD21  | 1.84                     | 0.60              |
| 31:BA:223:A:H62    | 78:BF:287:ARG:HH21 | 1.48                     | 0.60              |
| 85:BQ:240:ARG:NH1  | 85:BQ:251:VAL:O    | 2.34                     | 0.60              |
| 1:Al:115:GLY:HA3   | 37:AJ:84:ASP:HB2   | 1.83                     | 0.60              |
| 2:BT:79:GLU:OE2    | 2:BT:103:ARG:NH2   | 2.34                     | 0.60              |
| 31:AA:724:U:OP1    | 36:AG:195:LYS:NZ   | 2.34                     | 0.60              |
| 75:BC:637:ALA:O    | 75:BC:641:ALA:CB   | 2.50                     | 0.60              |
| 8:Ba:389:LEU:H     | 31:BA:725:C:H5     | 1.50                     | 0.59              |
| 24:Bq:73:MET:HE1   | 81:BK:94:ALA:HA    | 1.83                     | 0.59              |
| 31:AA:640:A:OP1    | 34:AE:242:ARG:NH1  | 2.35                     | 0.59              |
| 59:Aj:16:ARG:HD3   | 59:Aj:19:ARG:HH22  | 1.66                     | 0.59              |
| 59:Aj:70:ARG:HH21  | 59:Aj:141:LEU:HD21 | 1.67                     | 0.59              |
| 67:B3:68:ILE:HD11  | 67:B3:122:LEU:HD13 | 1.84                     | 0.59              |
| 84:BP:14:ASP:OD1   | 84:BP:17:ARG:NH1   | 2.35                     | 0.59              |
| 10:Bc:204:ARG:NH2  | 10:Bc:276:GLU:OE2  | 2.35                     | 0.59              |
| 17:Bj:147:THR:HG22 | 17:Bj:253:VAL:HG22 | 1.84                     | 0.59              |
| 31:AA:866:U:OP1    | 83:BO:78:ARG:NH2   | 2.35                     | 0.59              |
| 34:AE:140:LEU:HD21 | 34:AE:160:ARG:HE   | 1.67                     | 0.59              |
| 45:AU:80:ARG:NH1   | 55:Af:112:ASP:OD2  | 2.33                     | 0.59              |
| 75:BC:556:LEU:HD11 | 75:BC:607:LEU:HB3  | 1.82                     | 0.59              |
| 83:BO:86:ILE:HA    | 83:BO:105:VAL:HG12 | 1.82                     | 0.59              |
| 10:Bc:210:ASP:OD2  | 10:Bc:268:ARG:NH1  | 2.35                     | 0.59              |
| 12:Be:21:TRP:O     | 12:Be:32:LYS:NZ    | 2.35                     | 0.59              |
| 24:Bq:119:ARG:NE   | 31:BA:529:G:OP1    | 2.34                     | 0.59              |
| 25:Bt:32:LYS:HE2   | 80:BJ:49:ALA:HB1   | 1.84                     | 0.59              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:AA:800:G:H2'    | 31:AA:801:A:C8     | 2.36                     | 0.59              |
| 53:Ae:436:GLU:HA   | 53:Ae:439:GLU:HG2  | 1.84                     | 0.59              |
| 80:BJ:168:LEU:HD22 | 80:BJ:174:LEU:HD22 | 1.84                     | 0.59              |
| 9:Bb:124:ARG:HH12  | 11:Bd:72:LEU:HG    | 1.67                     | 0.59              |
| 17:Bj:140:ALA:HA   | 17:Bj:143:LYS:HE2  | 1.85                     | 0.59              |
| 31:AA:285:C:N4     | 39:AL:43:LYS:O     | 2.35                     | 0.59              |
| 40:AN:41:ARG:NH1   | 58:Ai:48:THR:O     | 2.35                     | 0.59              |
| 75:BC:65:ARG:NH1   | 75:BC:300:ALA:O    | 2.35                     | 0.59              |
| 29:Bw:49:ALA:O     | 29:Bw:61:ARG:NH1   | 2.35                     | 0.59              |
| 75:BC:203:ILE:HD13 | 75:BC:217:LEU:HD21 | 1.84                     | 0.59              |
| 1:AI:389:ARG:NH1   | 31:AA:789:C:OP1    | 2.35                     | 0.59              |
| 9:Bb:130:ILE:HD11  | 87:BS:116:LEU:HD13 | 1.85                     | 0.59              |
| 9:Bb:240:ILE:HD12  | 9:Bb:245:VAL:HA    | 1.84                     | 0.59              |
| 31:BA:62:C:OP1     | 79:BI:76:ARG:NH1   | 2.36                     | 0.59              |
| 9:Bb:374:GLU:HG3   | 26:Bu:140:ARG:HG2  | 1.84                     | 0.59              |
| 18:Bk:93:ILE:HB    | 18:Bk:157:VAL:HG23 | 1.85                     | 0.59              |
| 28:B0:92:LEU:HD13  | 87:BS:66:ARG:HE    | 1.66                     | 0.59              |
| 46:AY:24:U:H2'     | 46:AY:25:C:C6      | 2.37                     | 0.59              |
| 71:B7:66:LYS:NZ    | 31:BA:254:G:O5'    | 2.36                     | 0.59              |
| 31:BA:1307:A:O3'   | 85:BQ:101:HIS:NE2  | 2.35                     | 0.59              |
| 75:BC:98:ARG:NH1   | 75:BC:506:GLN:OE1  | 2.34                     | 0.59              |
| 75:BC:130:GLU:OE1  | 75:BC:133:ARG:NH2  | 2.35                     | 0.59              |
| 55:Af:153:ARG:NH2  | 55:Af:157:ALA:O    | 2.36                     | 0.59              |
| 56:Ag:317:LYS:NZ   | 56:Ag:327:LEU:O    | 2.29                     | 0.59              |
| 65:LL:151:SER:O    | 65:LL:154:GLN:NE2  | 2.36                     | 0.59              |
| 70:B6:63:ARG:NH1   | 31:BA:1245:G:OP1   | 2.36                     | 0.59              |
| 31:BA:215:A:OP1    | 78:BF:92:ARG:NH1   | 2.32                     | 0.59              |
| 31:BA:1513:U:OP2   | 31:BA:1525:C:N4    | 2.35                     | 0.59              |
| 31:BA:1559:A:OP2   | 77:BE:212:GLY:N    | 2.35                     | 0.59              |
| 79:BI:144:LYS:HG2  | 79:BI:147:ARG:HH12 | 1.68                     | 0.59              |
| 31:AA:621:A:OP2    | 33:AC:36:LYS:N     | 2.36                     | 0.59              |
| 15:Bh:33:LYS:NZ    | 31:BA:106:C:OP1    | 2.34                     | 0.59              |
| 31:AA:799:A:H2'    | 31:AA:800:G:H8     | 1.68                     | 0.59              |
| 36:AG:140:ASN:ND2  | 36:AG:143:THR:OG1  | 2.35                     | 0.59              |
| 8:Ba:173:ARG:NH2   | 31:BA:727:A:OP1    | 2.36                     | 0.58              |
| 8:Ba:229:ARG:HH21  | 8:Ba:288:PRO:HG3   | 1.68                     | 0.58              |
| 10:Bc:318:LYS:NZ   | 86:BR:156:ASP:OD2  | 2.34                     | 0.58              |
| 56:Ag:198:LEU:HA   | 56:Ag:221:LEU:HB3  | 1.85                     | 0.58              |
| 65:GL:70:ASP:HB3   | 65:HL:67:LEU:HD21  | 1.84                     | 0.58              |
| 67:B3:148:ARG:HB3  | 67:B3:151:LEU:HD21 | 1.83                     | 0.58              |
| 31:BA:81:G:N2      | 31:BA:85:A:OP2     | 2.33                     | 0.58              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 75:BC:175:LYS:HD3  | 75:BC:178:ARG:HH11 | 1.68                     | 0.58              |
| 14:Bg:78:GLU:HG2   | 14:Bg:84:VAL:HG22  | 1.85                     | 0.58              |
| 31:AA:847:C:N4     | 47:AX:6:G:OP1      | 2.36                     | 0.58              |
| 56:Ag:323:LEU:HD13 | 60:Ak:306:ASP:HB2  | 1.84                     | 0.58              |
| 31:BA:1383:G:O3'   | 83:BO:81:LYS:NZ    | 2.35                     | 0.58              |
| 7:BY:81:ARG:HD3    | 7:BY:81:ARG:H      | 1.67                     | 0.58              |
| 17:Bj:151:ARG:HG2  | 17:Bj:152:LYS:HG3  | 1.85                     | 0.58              |
| 25:Bt:42:GLU:OE2   | 67:B3:114:LYS:NZ   | 2.36                     | 0.58              |
| 28:B0:92:LEU:HB3   | 87:BS:66:ARG:HH21  | 1.67                     | 0.58              |
| 29:Bw:151:LEU:HD23 | 29:Bw:153:ARG:HH21 | 1.68                     | 0.58              |
| 31:AA:29:A:H2'     | 31:AA:30:A:C8      | 2.37                     | 0.58              |
| 31:AA:72:A:H2'     | 31:AA:73:G:C8      | 2.38                     | 0.58              |
| 31:AA:578:G:H3'    | 31:AA:579:A:H8     | 1.68                     | 0.58              |
| 31:BA:1418:G:N2    | 31:BA:1421:A:OP2   | 2.34                     | 0.58              |
| 83:BO:57:CYS:SG    | 83:BO:58:ILE:N     | 2.76                     | 0.58              |
| 8:Ba:353:GLN:HE22  | 8:Ba:379:ASP:H     | 1.50                     | 0.58              |
| 24:Bq:68:LEU:HD22  | 24:Bq:73:MET:HE2   | 1.85                     | 0.58              |
| 31:AA:77:G:OP1     | 59:Aj:3:ARG:NH2    | 2.36                     | 0.58              |
| 31:AA:740:U:OP1    | 36:AG:197:ARG:NH2  | 2.36                     | 0.58              |
| 64:Ap:213:LEU:HG   | 64:Ap:217:ARG:HE   | 1.68                     | 0.58              |
| 31:BA:642:G:H3'    | 31:BA:643:A:H8     | 1.68                     | 0.58              |
| 83:BO:89:HIS:HD2   | 83:BO:91:MET:H     | 1.51                     | 0.58              |
| 16:Bi:165:THR:HG23 | 16:Bi:167:ASN:H    | 1.69                     | 0.58              |
| 63:Ao:231:HIS:O    | 63:Ao:271:LYS:NZ   | 2.28                     | 0.58              |
| 6:BX:68:VAL:HG22   | 6:BX:97:VAL:HG12   | 1.85                     | 0.58              |
| 31:AA:759:U:H5''   | 58:Ai:29:LYS:HE3   | 1.84                     | 0.58              |
| 49:Aa:348:HIS:HD2  | 49:Aa:351:LYS:HB2  | 1.68                     | 0.58              |
| 51:Ac:112:THR:HA   | 51:Ac:115:LYS:HE3  | 1.84                     | 0.58              |
| 80:BJ:101:HIS:HB3  | 80:BJ:150:HIS:HB3  | 1.86                     | 0.58              |
| 87:BS:90:ILE:H     | 87:BS:107:THR:HG1  | 1.49                     | 0.58              |
| 16:Bi:90:PRO:HB2   | 16:Bi:269:TRP:HH2  | 1.69                     | 0.58              |
| 20:Bm:98:LYS:NZ    | 20:Bm:121:MET:O    | 2.35                     | 0.58              |
| 29:Bw:397:GLU:HG2  | 29:Bw:398:THR:HG22 | 1.85                     | 0.58              |
| 30:Bx:63:PRO:HG2   | 30:Bx:66:PRO:HG3   | 1.86                     | 0.58              |
| 65:LL:134:LEU:HB2  | 65:LL:172:ILE:HD11 | 1.86                     | 0.58              |
| 80:BJ:123:MET:HB2  | 80:BJ:152:LEU:HD11 | 1.86                     | 0.58              |
| 85:BQ:218:ILE:HG23 | 85:BQ:223:MET:HB2  | 1.86                     | 0.58              |
| 16:Bi:94:ASP:OD2   | 16:Bi:108:ARG:NH2  | 2.37                     | 0.58              |
| 16:Bi:267:PRO:HG2  | 16:Bi:270:ALA:HB2  | 1.84                     | 0.58              |
| 21:Bn:95:LYS:NZ    | 31:BA:64:C:O2'     | 2.33                     | 0.58              |
| 23:Bp:40:GLU:HA    | 23:Bp:43:ARG:HD3   | 1.85                     | 0.58              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 26:Bu:96:SER:O     | 26:Bu:145:ASN:ND2  | 2.37                     | 0.58              |
| 31:AA:767:U:HO2'   | 31:AA:806:A:HO2'   | 1.47                     | 0.58              |
| 37:AJ:89:ASP:OD1   | 37:AJ:141:ARG:NH2  | 2.36                     | 0.58              |
| 31:BA:388:A:H2'    | 31:BA:389:A:H8     | 1.68                     | 0.58              |
| 31:BA:842:U:OP2    | 31:BA:871:A:N6     | 2.22                     | 0.58              |
| 84:BP:261:ASP:HB3  | 84:BP:264:GLN:HB2  | 1.85                     | 0.58              |
| 2:BT:269:MET:SD    | 86:BR:79:TRP:NE1   | 2.77                     | 0.58              |
| 31:AA:641:A:H2'    | 31:AA:642:G:H8     | 1.69                     | 0.58              |
| 34:AE:134:GLU:OE2  | 34:AE:165:GLN:NE2  | 2.37                     | 0.58              |
| 42:AP:42:PRO:HG2   | 42:AP:45:GLY:HA3   | 1.86                     | 0.58              |
| 46:AV:40:A:H2'     | 46:AV:41:A:C8      | 2.39                     | 0.58              |
| 69:B5:140:GLN:NE2  | 69:B5:176:GLU:O    | 2.36                     | 0.58              |
| 71:B7:88:LYS:NZ    | 31:BA:127:G:OP2    | 2.33                     | 0.58              |
| 31:BA:197:U:H2'    | 31:BA:198:U:C6     | 2.38                     | 0.58              |
| 5:BW:147:ARG:O     | 31:BA:2:C:O2'      | 2.16                     | 0.58              |
| 7:BY:34:LYS:NZ     | 31:BA:138:A:OP1    | 2.37                     | 0.58              |
| 21:Bn:113:ARG:NH1  | 31:BA:348:G:O6     | 2.34                     | 0.58              |
| 25:Bt:31:ALA:HB1   | 80:BJ:46:LYS:HE3   | 1.86                     | 0.58              |
| 31:AA:767:U:O2'    | 31:AA:806:A:O2'    | 2.20                     | 0.58              |
| 31:AA:803:U:OP1    | 40:AN:89:ASN:ND2   | 2.35                     | 0.58              |
| 55:Af:105:ILE:HG12 | 55:Af:115:ILE:HG12 | 1.84                     | 0.58              |
| 68:B4:60:GLN:NE2   | 68:B4:79:PRO:O     | 2.32                     | 0.58              |
| 31:BA:1131:U:H2'   | 31:BA:1132:G:H8    | 1.69                     | 0.58              |
| 11:Bd:153:LYS:HD3  | 11:Bd:154:VAL:H    | 1.69                     | 0.57              |
| 49:Aa:100:ILE:HG23 | 49:Aa:321:SER:HB3  | 1.85                     | 0.57              |
| 26:Bu:107:ALA:O    | 26:Bu:115:ARG:NH2  | 2.36                     | 0.57              |
| 30:Bx:72:ILE:HG23  | 30:Bx:77:LEU:HB2   | 1.86                     | 0.57              |
| 31:AA:463:U:O4     | 31:AA:464:A:N6     | 2.37                     | 0.57              |
| 31:AA:708:A:H3'    | 31:AA:709:A:H8     | 1.69                     | 0.57              |
| 33:AC:136:VAL:HG23 | 33:AC:153:LEU:HD23 | 1.85                     | 0.57              |
| 41:AO:69:PRO:HD2   | 41:AO:72:MET:HG2   | 1.86                     | 0.57              |
| 51:Ac:91:GLU:OE1   | 52:Ad:120:ARG:NH2  | 2.37                     | 0.57              |
| 52:Ad:112:GLU:OE2  | 52:Ad:115:ARG:NH2  | 2.37                     | 0.57              |
| 53:Ae:328:LYS:HB3  | 53:Ae:368:LEU:HD13 | 1.86                     | 0.57              |
| 66:B2:96:SER:OG    | 66:B2:99:ASP:OD1   | 2.23                     | 0.57              |
| 31:BA:916:C:H2'    | 31:BA:917:G:H8     | 1.69                     | 0.57              |
| 31:BA:1336:A:H2'   | 31:BA:1337:G:H8    | 1.69                     | 0.57              |
| 80:BJ:99:CYS:SG    | 80:BJ:100:GLN:N    | 2.77                     | 0.57              |
| 81:BK:17:SER:N     | 81:BK:72:VAL:O     | 2.37                     | 0.57              |
| 31:AA:344:G:O6     | 38:AK:124:LYS:NZ   | 2.31                     | 0.57              |
| 31:BA:114:A:N3     | 31:BA:116:A:O2'    | 2.36                     | 0.57              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:BA:1281:A:O2'   | 31:BA:1283:U:O4    | 2.20                     | 0.57              |
| 75:BC:406:MET:SD   | 75:BC:406:MET:N    | 2.77                     | 0.57              |
| 4:BV:173:LYS:NZ    | 31:BA:477:A:O3'    | 2.37                     | 0.57              |
| 6:BX:12:LEU:HD22   | 8:Ba:85:PRO:HD3    | 1.86                     | 0.57              |
| 8:Ba:35:VAL:HB     | 8:Ba:38:THR:HG22   | 1.87                     | 0.57              |
| 8:Ba:350:ARG:HH12  | 8:Ba:381:LEU:HD23  | 1.70                     | 0.57              |
| 15:Bh:60:ARG:NH1   | 15:Bh:60:ARG:O     | 2.36                     | 0.57              |
| 31:AA:343:U:H3     | 31:AA:350:A:H61    | 1.53                     | 0.57              |
| 53:Ae:80:TRP:HH2   | 53:Ae:151:THR:HG23 | 1.67                     | 0.57              |
| 31:BA:165:A:H2'    | 31:BA:166:A:C8     | 2.39                     | 0.57              |
| 9:Bb:136:ARG:NH1   | 87:BS:138:GLU:OE1  | 2.37                     | 0.57              |
| 29:Bw:215:HIS:ND1  | 31:BA:757:A:OP1    | 2.36                     | 0.57              |
| 33:AC:148:LYS:NZ   | 63:Ao:140:LEU:O    | 2.33                     | 0.57              |
| 59:Aj:78:ARG:NH2   | 59:Aj:142:VAL:O    | 2.37                     | 0.57              |
| 68:B4:58:VAL:HB    | 68:B4:64:THR:HG22  | 1.86                     | 0.57              |
| 72:B8:123:LEU:HD11 | 72:B8:147:PHE:HB3  | 1.86                     | 0.57              |
| 8:Ba:63:LYS:NZ     | 8:Ba:67:MET:SD     | 2.67                     | 0.57              |
| 14:Bg:48:GLU:OE2   | 25:Bt:101:TRP:NE1  | 2.33                     | 0.57              |
| 29:Bw:147:GLU:HG3  | 29:Bw:170:PHE:HA   | 1.85                     | 0.57              |
| 31:AA:959:U:OP2    | 45:AU:61:ARG:NH1   | 2.37                     | 0.57              |
| 40:AN:54:ILE:HG21  | 40:AN:75:ILE:HB    | 1.86                     | 0.57              |
| 46:AV:4:A:H2'      | 46:AV:5:A:H8       | 1.68                     | 0.57              |
| 31:BA:763:C:OP2    | 31:BA:765:C:N4     | 2.36                     | 0.57              |
| 31:BA:918:U:H2'    | 31:BA:919:G:H8     | 1.69                     | 0.57              |
| 78:BF:66:ILE:HD11  | 78:BF:80:THR:HB    | 1.86                     | 0.57              |
| 21:Bn:32:PHE:HD1   | 31:BA:199:A:H5''   | 1.68                     | 0.57              |
| 31:AA:915:G:H2'    | 31:AA:916:A:C8     | 2.40                     | 0.57              |
| 32:AB:192:ILE:HD12 | 32:AB:211:ALA:HB2  | 1.86                     | 0.57              |
| 49:Aa:101:LEU:HD22 | 49:Aa:291:GLY:HA2  | 1.87                     | 0.57              |
| 11:Bd:129:ARG:HB3  | 18:Bk:184:LEU:HB3  | 1.86                     | 0.57              |
| 31:AA:249:C:N4     | 39:AL:117:ASP:OD1  | 2.34                     | 0.57              |
| 40:AN:84:PRO:HG3   | 58:Ai:43:ALA:HB2   | 1.86                     | 0.57              |
| 31:BA:792:G:OP1    | 77:BE:238:ARG:N    | 2.38                     | 0.57              |
| 31:BA:843:C:O2'    | 76:BD:258:ILE:O    | 2.19                     | 0.57              |
| 29:Bw:154:LYS:NZ   | 31:BA:741:A:OP2    | 2.37                     | 0.57              |
| 29:Bw:394:PRO:O    | 29:Bw:408:ASN:ND2  | 2.35                     | 0.57              |
| 31:AA:17:G:H2'     | 31:AA:18:G:C8      | 2.40                     | 0.57              |
| 33:AC:133:TYR:HA   | 33:AC:136:VAL:HG12 | 1.87                     | 0.57              |
| 33:AC:163:VAL:HG21 | 33:AC:167:ILE:HD12 | 1.87                     | 0.57              |
| 35:AF:90:ARG:NH1   | 44:AR:117:ILE:O    | 2.37                     | 0.57              |
| 37:AJ:123:SER:HB3  | 37:AJ:127:PHE:HB2  | 1.85                     | 0.57              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 52:Ad:62:GLN:NE2   | 52:Ad:65:GLN:OE1  | 2.38                     | 0.57              |
| 67:B3:104:PRO:HA   | 67:B3:107:ASN:HB2 | 1.87                     | 0.57              |
| 31:BA:803:A:N3     | 31:BA:805:C:N4    | 2.51                     | 0.57              |
| 31:BA:1066:A:H2'   | 31:BA:1067:G:H8   | 1.70                     | 0.57              |
| 9:Bb:124:ARG:HH22  | 11:Bd:72:LEU:HD23 | 1.68                     | 0.57              |
| 24:Bq:121:LEU:HD11 | 85:BQ:35:PRO:HA   | 1.87                     | 0.57              |
| 31:AA:913:G:H2'    | 31:AA:914:A:H8    | 1.69                     | 0.57              |
| 56:Ag:67:TYR:HH    | 56:Ag:139:HIS:HD1 | 1.49                     | 0.57              |
| 31:BA:198:U:H2'    | 31:BA:199:A:C8    | 2.39                     | 0.57              |
| 3:BU:13:ARG:NH2    | 31:BA:200:A:O3'   | 2.38                     | 0.56              |
| 3:BU:34:ARG:NH2    | 31:BA:1014:A:OP1  | 2.38                     | 0.56              |
| 8:Ba:295:GLU:HB2   | 8:Ba:348:ASP:HA   | 1.87                     | 0.56              |
| 31:AA:765:A:C6     | 31:AA:805:G:N2    | 2.73                     | 0.56              |
| 42:AP:88:GLU:OE1   | 52:Ad:63:TYR:OH   | 2.23                     | 0.56              |
| 60:Ak:216:LEU:O    | 60:Ak:220:ASN:ND2 | 2.38                     | 0.56              |
| 8:Ba:249:LYS:HE2   | 8:Ba:370:VAL:HG22 | 1.87                     | 0.56              |
| 15:Bh:45:LEU:HD22  | 31:BA:147:U:H4'   | 1.87                     | 0.56              |
| 31:AA:168:A:O2'    | 31:AA:169:A:O4'   | 2.19                     | 0.56              |
| 31:AA:194:U:H2'    | 31:AA:195:G:C8    | 2.40                     | 0.56              |
| 31:AA:226:G:H2'    | 31:AA:227:A:H8    | 1.68                     | 0.56              |
| 31:AA:728:U:H2'    | 31:AA:729:A:C8    | 2.40                     | 0.56              |
| 69:B5:138:ARG:HA   | 69:B5:141:MET:HG2 | 1.86                     | 0.56              |
| 31:BA:344:U:H2'    | 31:BA:345:G:H8    | 1.70                     | 0.56              |
| 31:BA:565:A:N6     | 31:BA:1314:U:OP1  | 2.37                     | 0.56              |
| 87:BS:68:TRP:CD1   | 87:BS:68:TRP:H    | 2.23                     | 0.56              |
| 1:AI:313:GLN:NE2   | 36:AG:79:ALA:O    | 2.38                     | 0.56              |
| 7:BY:25:ARG:HB3    | 7:BY:28:SER:HB3   | 1.87                     | 0.56              |
| 14:Bg:95:GLU:N     | 14:Bg:95:GLU:OE1  | 2.38                     | 0.56              |
| 31:AA:550:G:N2     | 31:AA:783:A:OP2   | 2.31                     | 0.56              |
| 35:AF:49:TYR:OH    | 35:AF:90:ARG:NH1  | 2.38                     | 0.56              |
| 36:AG:171:PRO:HG3  | 36:AG:234:ARG:HA  | 1.87                     | 0.56              |
| 56:Ag:311:GLN:NE2  | 56:Ag:318:PRO:O   | 2.39                     | 0.56              |
| 60:Ak:191:LYS:NZ   | 60:Ak:237:LYS:O   | 2.38                     | 0.56              |
| 72:B8:104:ARG:NH2  | 72:B8:160:LYS:O   | 2.39                     | 0.56              |
| 31:BA:6:A:H2'      | 31:BA:7:G:C4      | 2.40                     | 0.56              |
| 31:BA:416:U:H2'    | 31:BA:417:G:C8    | 2.41                     | 0.56              |
| 31:BA:644:G:N2     | 31:BA:1008:A:OP2  | 2.37                     | 0.56              |
| 31:BA:709:A:H2'    | 31:BA:710:A:H8    | 1.70                     | 0.56              |
| 31:BA:1411:G:O6    | 31:BA:1430:G:N1   | 2.38                     | 0.56              |
| 85:BQ:240:ARG:NH2  | 85:BQ:246:TYR:OH  | 2.38                     | 0.56              |
| 1:AI:276:LYS:H     | 1:AI:347:LEU:HD23 | 1.71                     | 0.56              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:Bb:75:ARG:HB3    | 9:Bb:80:GLU:HB3    | 1.87                     | 0.56              |
| 17:Bj:129:LEU:O    | 17:Bj:132:LYS:NZ   | 2.39                     | 0.56              |
| 37:AJ:75:ARG:H     | 37:AJ:175:THR:HB   | 1.69                     | 0.56              |
| 46:AV:7:G:O2'      | 46:AV:45:G:O4'     | 2.23                     | 0.56              |
| 57:Ah:379:LEU:HD13 | 57:Ah:386:LEU:HB2  | 1.88                     | 0.56              |
| 60:Ak:190:LYS:O    | 60:Ak:194:LYS:NZ   | 2.36                     | 0.56              |
| 66:B2:204:MET:HE3  | 66:B2:205:PRO:HD2  | 1.87                     | 0.56              |
| 69:B5:93:ARG:NH2   | 31:BA:642:G:OP1    | 2.38                     | 0.56              |
| 31:BA:789:A:O2'    | 77:BE:215:PHE:O    | 2.20                     | 0.56              |
| 87:BS:173:ARG:NH1  | 87:BS:174:GLU:O    | 2.39                     | 0.56              |
| 31:AA:714:U:H2'    | 31:AA:715:G:H8     | 1.70                     | 0.56              |
| 55:Af:141:VAL:HA   | 55:Af:173:LEU:HA   | 1.87                     | 0.56              |
| 59:Aj:52:MET:SD    | 64:Ap:223:ARG:NH2  | 2.79                     | 0.56              |
| 69:B5:95:ARG:NH1   | 31:BA:157:A:OP2    | 2.39                     | 0.56              |
| 31:BA:436:U:H2'    | 31:BA:437:A:H8     | 1.71                     | 0.56              |
| 31:BA:740:U:H2'    | 31:BA:741:A:C8     | 2.40                     | 0.56              |
| 3:BU:97:LEU:HA     | 4:BV:109:GLN:HE22  | 1.71                     | 0.56              |
| 9:Bb:351:HIS:ND1   | 31:BA:1196:G:OP1   | 2.37                     | 0.56              |
| 11:Bd:24:LEU:HD21  | 18:Bk:211:LEU:HB2  | 1.88                     | 0.56              |
| 30:Bx:193:LEU:N    | 31:BA:574:A:O2'    | 2.34                     | 0.56              |
| 31:AA:62:C:N4      | 31:AA:63:G:O6      | 2.39                     | 0.56              |
| 31:AA:202:A:N1     | 59:Aj:53:ARG:NH2   | 2.54                     | 0.56              |
| 29:Bw:265:LEU:HD23 | 29:Bw:267:LEU:HG   | 1.86                     | 0.56              |
| 29:Bw:399:ILE:HG22 | 29:Bw:404:VAL:HA   | 1.88                     | 0.56              |
| 31:AA:56:U:H1'     | 31:AA:198:C:H1'    | 1.88                     | 0.56              |
| 31:AA:941:U:H2'    | 31:AA:942:G:C8     | 2.40                     | 0.56              |
| 46:AY:25:C:H2'     | 46:AY:26:G:C8      | 2.41                     | 0.56              |
| 46:AY:60:C:H2'     | 46:AY:61:C:C6      | 2.40                     | 0.56              |
| 63:Ao:627:PRO:HB3  | 63:Ao:659:THR:HG21 | 1.87                     | 0.56              |
| 64:Ap:93:MET:HE2   | 64:Ap:96:ARG:HG2   | 1.87                     | 0.56              |
| 69:B5:156:THR:HG22 | 69:B5:173:ARG:HB3  | 1.86                     | 0.56              |
| 31:BA:671:C:N4     | 31:BA:672:G:O6     | 2.39                     | 0.56              |
| 31:BA:1463:A:C6    | 75:BC:704:ARG:HB2  | 2.41                     | 0.56              |
| 87:BS:39:VAL:HB    | 87:BS:42:GLU:HB2   | 1.87                     | 0.56              |
| 17:Bj:67:GLN:HB3   | 68:B4:41:LEU:HD11  | 1.88                     | 0.56              |
| 18:Bk:97:ALA:HB2   | 18:Bk:182:VAL:HG12 | 1.87                     | 0.56              |
| 31:AA:389:A:H5''   | 41:AO:101:GLN:HB2  | 1.87                     | 0.56              |
| 57:Ah:335:LYS:HA   | 57:Ah:340:ARG:HG3  | 1.88                     | 0.56              |
| 31:BA:289:U:H2'    | 31:BA:290:A:H8     | 1.69                     | 0.56              |
| 31:BA:1309:U:H2'   | 31:BA:1310:A:C8    | 2.41                     | 0.56              |
| 33:AC:113:ARG:NH2  | 37:AJ:166:GLU:OE1  | 2.39                     | 0.56              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 52:Ad:45:PRO:HB3   | 59:Aj:53:ARG:HH21  | 1.70                     | 0.56              |
| 61:Am:40:LYS:HD3   | 61:Am:41:GLY:H     | 1.71                     | 0.56              |
| 31:BA:414:A:H3'    | 31:BA:415:A:H8     | 1.71                     | 0.56              |
| 31:BA:995:C:OP1    | 86:BR:13:ARG:NH2   | 2.39                     | 0.56              |
| 75:BC:53:ALA:HB2   | 75:BC:144:VAL:HB   | 1.87                     | 0.56              |
| 6:BX:14:ASN:OD1    | 7:BY:210:HIS:ND1   | 2.38                     | 0.56              |
| 15:Bh:80:GLN:O     | 15:Bh:210:ARG:NH2  | 2.38                     | 0.56              |
| 17:Bj:273:ARG:HA   | 17:Bj:276:LEU:HB3  | 1.87                     | 0.56              |
| 31:AA:418:C:O2'    | 38:AK:189:ARG:O    | 2.24                     | 0.56              |
| 33:AC:50:PRO:HB3   | 33:AC:167:ILE:HG13 | 1.88                     | 0.56              |
| 53:Ae:280:LEU:HD11 | 53:Ae:293:PRO:HB3  | 1.87                     | 0.56              |
| 54:B1:167:LEU:HD21 | 54:B1:202:GLU:HB3  | 1.87                     | 0.56              |
| 60:Ak:165:ILE:HD11 | 63:Ao:135:PRO:HD3  | 1.87                     | 0.56              |
| 31:BA:570:A:H2'    | 31:BA:571:A:C8     | 2.40                     | 0.56              |
| 74:BB:40:U:H2'     | 74:BB:41:G:C8      | 2.41                     | 0.56              |
| 85:BQ:204:GLU:OE2  | 85:BQ:208:ASN:ND2  | 2.39                     | 0.56              |
| 7:BY:122:LEU:HD23  | 7:BY:133:VAL:HG21  | 1.88                     | 0.55              |
| 31:AA:680:U:OP1    | 34:AE:114:ARG:NH2  | 2.39                     | 0.55              |
| 34:AE:243:VAL:HG11 | 34:AE:268:PHE:HE1  | 1.70                     | 0.55              |
| 35:AF:22:LEU:HD13  | 35:AF:39:LEU:HD21  | 1.87                     | 0.55              |
| 43:AQ:69:LEU:HD12  | 43:AQ:70:PRO:HD2   | 1.87                     | 0.55              |
| 57:Ah:307:ILE:HB   | 60:Ak:159:VAL:HG12 | 1.89                     | 0.55              |
| 31:BA:52:A:O2'     | 31:BA:349:A:N3     | 2.37                     | 0.55              |
| 31:BA:619:C:H2'    | 31:BA:620:A:H8     | 1.71                     | 0.55              |
| 31:BA:771:U:H2'    | 31:BA:772:G:C8     | 2.40                     | 0.55              |
| 31:AA:798:A:H2'    | 31:AA:799:A:H8     | 1.70                     | 0.55              |
| 31:AA:873:A:OP1    | 41:AO:225:LYS:NZ   | 2.39                     | 0.55              |
| 41:AO:155:ARG:NE   | 41:AO:159:MET:SD   | 2.80                     | 0.55              |
| 49:Aa:185:TYR:HB2  | 51:Ac:125:HIS:HE1  | 1.71                     | 0.55              |
| 1:AI:294:ILE:HG23  | 1:AI:329:MET:HG3   | 1.88                     | 0.55              |
| 31:AA:15:C:H4'     | 34:AE:300:ARG:HG3  | 1.88                     | 0.55              |
| 32:AB:196:HIS:NE2  | 32:AB:239:ASP:O    | 2.39                     | 0.55              |
| 60:Ak:143:GLU:OE1  | 60:Ak:143:GLU:N    | 2.38                     | 0.55              |
| 4:BV:143:ASP:OD2   | 15:Bh:310:ASN:ND2  | 2.39                     | 0.55              |
| 11:Bd:42:GLU:OE2   | 11:Bd:155:TYR:OH   | 2.22                     | 0.55              |
| 30:Bx:81:TYR:HB3   | 30:Bx:88:LEU:HD23  | 1.88                     | 0.55              |
| 31:AA:115:A:H5''   | 41:AO:204:TRP:HD1  | 1.71                     | 0.55              |
| 65:DL:90:LEU:HD23  | 80:BJ:214:LEU:HB2  | 1.89                     | 0.55              |
| 67:B3:88:MET:SD    | 31:BA:417:G:N2     | 2.79                     | 0.55              |
| 77:BE:69:ASN:HD21  | 77:BE:154:HIS:HE1  | 1.53                     | 0.55              |
| 15:Bh:264:THR:H    | 82:BN:140:ASN:HD21 | 1.54                     | 0.55              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:Bt:15:ARG:NH1   | 31:BA:1025:A:OP1   | 2.40                     | 0.55              |
| 31:AA:313:A:O2'    | 31:AA:314:A:O4'    | 2.25                     | 0.55              |
| 42:AP:118:VAL:HG21 | 64:Ap:236:PRO:HB2  | 1.89                     | 0.55              |
| 51:Ac:91:GLU:HB2   | 52:Ad:120:ARG:HH21 | 1.71                     | 0.55              |
| 52:Ad:166:THR:O    | 52:Ad:176:ARG:NH2  | 2.40                     | 0.55              |
| 57:Ah:284:ARG:HH22 | 63:Ao:457:ARG:HH11 | 1.54                     | 0.55              |
| 76:BD:198:GLU:OE2  | 76:BD:204:GLY:N    | 2.38                     | 0.55              |
| 1:AI:116:LEU:O     | 1:AI:122:ARG:NH2   | 2.40                     | 0.55              |
| 9:Bb:364:ARG:NH1   | 72:B8:146:GLU:OE2  | 2.34                     | 0.55              |
| 31:AA:581:A:H61    | 31:AA:806:A:H3'    | 1.70                     | 0.55              |
| 56:Ag:107:LEU:HD13 | 56:Ag:140:ILE:HG13 | 1.88                     | 0.55              |
| 31:BA:219:A:H2'    | 31:BA:220:G:H8     | 1.71                     | 0.55              |
| 31:BA:1569:A:N1    | 77:BE:69:ASN:ND2   | 2.54                     | 0.55              |
| 18:Bk:179:PRO:HD2  | 18:Bk:182:VAL:HG21 | 1.88                     | 0.55              |
| 29:Bw:308:GLN:HG2  | 31:BA:748:A:H8     | 1.71                     | 0.55              |
| 38:AK:160:ARG:NH2  | 38:AK:179:ASP:OD1  | 2.37                     | 0.55              |
| 49:Aa:347:LEU:HD21 | 49:Aa:372:GLN:HE22 | 1.69                     | 0.55              |
| 57:Ah:345:LEU:HB3  | 58:Ai:34:VAL:HG22  | 1.89                     | 0.55              |
| 31:BA:344:U:H2'    | 31:BA:345:G:C8     | 2.41                     | 0.55              |
| 85:BQ:98:HIS:HB3   | 85:BQ:151:VAL:HG12 | 1.89                     | 0.55              |
| 15:Bh:45:LEU:HD13  | 31:BA:147:U:H5''   | 1.89                     | 0.55              |
| 15:Bh:215:ILE:HG23 | 15:Bh:219:LEU:HD12 | 1.88                     | 0.55              |
| 22:Bo:50:SER:HA    | 22:Bo:57:ALA:HB2   | 1.89                     | 0.55              |
| 31:AA:828:U:H2'    | 31:AA:829:G:H8     | 1.71                     | 0.55              |
| 35:AF:37:ARG:NH2   | 35:AF:69:TYR:OH    | 2.37                     | 0.55              |
| 43:AQ:17:VAL:HG22  | 43:AQ:28:VAL:HG22  | 1.89                     | 0.55              |
| 31:BA:527:U:H2'    | 31:BA:529:G:N7     | 2.22                     | 0.55              |
| 4:BV:198:ARG:NH2   | 14:Bg:13:SER:OG    | 2.40                     | 0.55              |
| 11:Bd:53:LYS:HB3   | 17:Bj:84:TYR:HB2   | 1.89                     | 0.55              |
| 17:Bj:55:ARG:NH2   | 17:Bj:152:LYS:O    | 2.39                     | 0.55              |
| 31:AA:75:A:N7      | 31:AA:146:U:C2     | 2.74                     | 0.55              |
| 33:AC:38:ARG:HG2   | 33:AC:43:ARG:HH21  | 1.72                     | 0.55              |
| 56:Ag:162:LYS:HD3  | 56:Ag:315:LEU:HD11 | 1.89                     | 0.55              |
| 31:BA:1137:A:H2'   | 31:BA:1138:G:C8    | 2.42                     | 0.55              |
| 75:BC:133:ARG:NH1  | 75:BC:358:PHE:O    | 2.37                     | 0.55              |
| 11:Bd:43:ASP:O     | 68:B4:46:ARG:NH1   | 2.40                     | 0.55              |
| 21:Bn:78:ILE:HG13  | 31:BA:16:A:H5''    | 1.89                     | 0.55              |
| 29:Bw:239:ARG:NH1  | 29:Bw:424:LYS:O    | 2.40                     | 0.55              |
| 34:AE:95:ALA:HB2   | 58:Ai:74:GLU:HB3   | 1.89                     | 0.55              |
| 73:B9:78:LEU:HD11  | 73:B9:85:TRP:HB3   | 1.89                     | 0.55              |
| 31:BA:245:A:HO2'   | 31:BA:1065:G:HO2'  | 1.47                     | 0.55              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:BA:996:U:OP2    | 86:BR:17:ARG:NH2   | 2.40                     | 0.55              |
| 84:BP:226:PRO:HA   | 84:BP:229:PHE:HD1  | 1.71                     | 0.55              |
| 31:AA:386:U:H2'    | 31:AA:387:C:H6     | 1.72                     | 0.54              |
| 31:AA:944:A:H5''   | 62:An:145:LYS:HZ1  | 1.72                     | 0.54              |
| 52:Ad:51:THR:HG21  | 64:Ap:228:SER:H    | 1.72                     | 0.54              |
| 55:Af:133:GLU:O    | 55:Af:136:GLN:NE2  | 2.40                     | 0.54              |
| 70:B6:21:MET:HG2   | 70:B6:29:SER:HB3   | 1.88                     | 0.54              |
| 70:B6:42:THR:HG23  | 70:B6:57:VAL:HG12  | 1.88                     | 0.54              |
| 75:BC:179:MET:HA   | 75:BC:208:GLU:HG3  | 1.89                     | 0.54              |
| 84:BP:203:ARG:NH2  | 84:BP:261:ASP:O    | 2.40                     | 0.54              |
| 8:Ba:135:LYS:HD2   | 8:Ba:239:VAL:HG23  | 1.89                     | 0.54              |
| 10:Bc:85:PRO:HG2   | 10:Bc:112:MET:HA   | 1.89                     | 0.54              |
| 15:Bh:262:GLY:HA2  | 82:BN:140:ASN:HA   | 1.90                     | 0.54              |
| 31:AA:441:U:H2'    | 31:AA:442:A:C8     | 2.42                     | 0.54              |
| 40:AN:105:ARG:HH21 | 58:Ai:47:GLU:HG2   | 1.71                     | 0.54              |
| 75:BC:111:TRP:CG   | 75:BC:112:LYS:H    | 2.24                     | 0.54              |
| 2:BT:117:LEU:HD22  | 2:BT:176:VAL:HG22  | 1.88                     | 0.54              |
| 26:Bu:52:SER:HB3   | 26:Bu:57:THR:HG21  | 1.89                     | 0.54              |
| 43:AQ:98:LYS:HE3   | 43:AQ:109:PRO:HA   | 1.89                     | 0.54              |
| 56:Ag:122:ARG:NH2  | 56:Ag:296:VAL:O    | 2.40                     | 0.54              |
| 56:Ag:221:LEU:HD11 | 56:Ag:242:VAL:HG23 | 1.89                     | 0.54              |
| 76:BD:128:ILE:HD12 | 76:BD:142:LEU:HG   | 1.90                     | 0.54              |
| 9:Bb:35:MET:HE3    | 9:Bb:36:PRO:HD2    | 1.90                     | 0.54              |
| 10:Bc:175:ALA:HB2  | 10:Bc:316:SER:HB2  | 1.89                     | 0.54              |
| 17:Bj:152:LYS:NZ   | 17:Bj:259:GLU:OE1  | 2.41                     | 0.54              |
| 27:Bv:35:GLN:O     | 27:Bv:64:HIS:NE2   | 2.36                     | 0.54              |
| 30:Bx:94:ARG:NH2   | 82:BN:176:TYR:OH   | 2.40                     | 0.54              |
| 31:AA:327:U:O2'    | 31:AA:328:A:N7     | 2.35                     | 0.54              |
| 31:AA:776:A:H2'    | 31:AA:777:A:C8     | 2.43                     | 0.54              |
| 31:AA:792:U:H2'    | 31:AA:793:A:H8     | 1.71                     | 0.54              |
| 42:AP:59:ASN:HD21  | 42:AP:63:GLU:HB2   | 1.72                     | 0.54              |
| 56:Ag:66:HIS:HB3   | 56:Ag:97:CYS:HB3   | 1.88                     | 0.54              |
| 59:Aj:30:ASP:N     | 59:Aj:30:ASP:OD1   | 2.40                     | 0.54              |
| 60:Ak:123:ARG:HG2  | 63:Ao:77:THR:HB    | 1.89                     | 0.54              |
| 31:BA:840:C:H2'    | 31:BA:841:A:C8     | 2.42                     | 0.54              |
| 77:BE:334:ASP:OD1  | 77:BE:335:GLU:N    | 2.39                     | 0.54              |
| 80:BJ:171:ILE:HD12 | 80:BJ:172:PRO:HD2  | 1.89                     | 0.54              |
| 6:BX:5:VAL:HG21    | 12:Be:135:ARG:HD2  | 1.89                     | 0.54              |
| 20:Bm:68:GLN:HE22  | 20:Bm:128:LEU:HD21 | 1.71                     | 0.54              |
| 31:AA:939:A:H2'    | 31:AA:940:C:C6     | 2.43                     | 0.54              |
| 31:BA:233:A:H2'    | 31:BA:234:G:C8     | 2.42                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:BA:1534:A:H2'   | 31:BA:1535:U:O4'   | 2.07                     | 0.54              |
| 2:BT:96:ARG:NH1    | 2:BT:285:GLU:OE1   | 2.41                     | 0.54              |
| 5:BW:77:GLN:H      | 5:BW:171:HIS:HD2   | 1.54                     | 0.54              |
| 9:Bb:50:LYS:O      | 9:Bb:52:ARG:NH1    | 2.40                     | 0.54              |
| 9:Bb:217:LEU:HD13  | 9:Bb:236:LEU:HD13  | 1.89                     | 0.54              |
| 9:Bb:267:ARG:HH21  | 87:BS:51:ARG:HG3   | 1.73                     | 0.54              |
| 31:AA:65:C:N4      | 31:AA:157:A:O2'    | 2.41                     | 0.54              |
| 31:AA:121:C:H2'    | 31:AA:122:C:C6     | 2.43                     | 0.54              |
| 31:AA:800:G:H2'    | 31:AA:801:A:H8     | 1.73                     | 0.54              |
| 35:AF:3:ARG:NH1    | 41:AO:98:MET:O     | 2.39                     | 0.54              |
| 50:Ab:86:ASP:OD1   | 55:Af:140:ARG:NH2  | 2.38                     | 0.54              |
| 65:CL:72:ALA:HA    | 65:FL:76:LEU:HB2   | 1.89                     | 0.54              |
| 31:BA:93:U:OP1     | 84:BP:196:ARG:NH1  | 2.40                     | 0.54              |
| 76:BD:111:ARG:NH1  | 76:BD:244:THR:OG1  | 2.41                     | 0.54              |
| 77:BE:103:LYS:NZ   | 77:BE:289:VAL:O    | 2.39                     | 0.54              |
| 17:Bj:258:GLU:OE1  | 17:Bj:258:GLU:N    | 2.39                     | 0.54              |
| 31:AA:675:A:OP1    | 33:AC:41:ARG:NH1   | 2.41                     | 0.54              |
| 57:Ah:366:GLU:O    | 57:Ah:370:ASN:ND2  | 2.40                     | 0.54              |
| 31:BA:1336:A:H2'   | 31:BA:1337:G:C8    | 2.42                     | 0.54              |
| 21:Bn:128:ARG:NH2  | 84:BP:62:ARG:O     | 2.40                     | 0.54              |
| 38:AK:99:ILE:HD11  | 38:AK:163:ALA:HB1  | 1.89                     | 0.54              |
| 49:Aa:179:VAL:HG11 | 49:Aa:214:MET:HE3  | 1.89                     | 0.54              |
| 49:Aa:194:ILE:HG13 | 49:Aa:211:ARG:HG3  | 1.88                     | 0.54              |
| 59:Aj:135:MET:SD   | 59:Aj:135:MET:N    | 2.79                     | 0.54              |
| 72:B8:113:ARG:NH2  | 31:BA:84:G:OP2     | 2.40                     | 0.54              |
| 31:BA:1131:U:H2'   | 31:BA:1132:G:C8    | 2.43                     | 0.54              |
| 31:BA:1414:C:N4    | 31:BA:1415:G:O6    | 2.41                     | 0.54              |
| 31:BA:1569:A:H62   | 77:BE:153:SER:HA   | 1.72                     | 0.54              |
| 7:BY:19:TYR:OH     | 7:BY:31:ASP:OD2    | 2.26                     | 0.54              |
| 11:Bd:138:ILE:H    | 68:B4:62:GLY:HA3   | 1.73                     | 0.54              |
| 29:Bw:128:GLU:HG2  | 29:Bw:422:ARG:HH21 | 1.73                     | 0.54              |
| 29:Bw:188:VAL:HG21 | 29:Bw:423:PRO:HD2  | 1.90                     | 0.54              |
| 31:AA:175:A:N3     | 31:AA:187:U:O2'    | 2.38                     | 0.54              |
| 36:AG:240:ARG:NH2  | 61:Am:44:THR:O     | 2.40                     | 0.54              |
| 61:Am:92:ASN:O     | 61:Am:103:LYS:NZ   | 2.33                     | 0.54              |
| 31:BA:439:A:OP1    | 85:BQ:73:ARG:NH1   | 2.41                     | 0.54              |
| 77:BE:100:ILE:HD11 | 77:BE:177:LYS:HB2  | 1.89                     | 0.54              |
| 14:Bg:65:VAL:HB    | 20:Bm:155:ILE:HG12 | 1.90                     | 0.54              |
| 49:Aa:92:PHE:O     | 49:Aa:98:GLN:NE2   | 2.34                     | 0.54              |
| 31:BA:611:U:H2'    | 31:BA:612:A:H8     | 1.72                     | 0.54              |
| 75:BC:64:GLU:OE1   | 75:BC:77:HIS:N     | 2.38                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 75:BC:171:THR:HB   | 75:BC:295:VAL:HG22 | 1.90                     | 0.54              |
| 76:BD:177:ALA:HB1  | 76:BD:245:VAL:HG11 | 1.88                     | 0.54              |
| 83:BO:114:PRO:HG3  | 83:BO:137:VAL:HA   | 1.90                     | 0.54              |
| 8:Ba:229:ARG:HE    | 8:Ba:231:ASN:HD21  | 1.56                     | 0.53              |
| 9:Bb:160:ASP:OD2   | 9:Bb:267:ARG:NH2   | 2.42                     | 0.53              |
| 11:Bd:19:ALA:O     | 11:Bd:23:ARG:HG2   | 2.08                     | 0.53              |
| 26:Bu:51:GLU:N     | 26:Bu:51:GLU:OE1   | 2.40                     | 0.53              |
| 28:B0:88:CYS:SG    | 31:BA:1207:C:O2'   | 2.66                     | 0.53              |
| 31:AA:8:U:O2'      | 31:AA:518:A:OP2    | 2.25                     | 0.53              |
| 31:AA:458:C:O2'    | 31:AA:460:A:OP2    | 2.25                     | 0.53              |
| 31:AA:603:U:H2'    | 31:AA:605:C:H4'    | 1.90                     | 0.53              |
| 31:AA:798:A:H2'    | 31:AA:799:A:C8     | 2.44                     | 0.53              |
| 33:AC:120:CYS:HB3  | 60:Ak:108:LEU:HD23 | 1.90                     | 0.53              |
| 51:Ac:51:ASN:ND2   | 51:Ac:95:ASN:OD1   | 2.41                     | 0.53              |
| 60:Ak:88:ARG:NH1   | 60:Ak:98:PRO:O     | 2.35                     | 0.53              |
| 65:LL:144:LYS:HE2  | 65:LL:191:VAL:HG12 | 1.89                     | 0.53              |
| 31:BA:1457:A:H61   | 31:BA:1468:A:H5'   | 1.73                     | 0.53              |
| 75:BC:128:THR:OG1  | 75:BC:161:GLN:NE2  | 2.38                     | 0.53              |
| 75:BC:594:CYS:HA   | 75:BC:604:LEU:HD12 | 1.89                     | 0.53              |
| 8:Ba:125:LYS:HA    | 8:Ba:253:LEU:HD11  | 1.91                     | 0.53              |
| 31:AA:154:C:H2'    | 31:AA:155:A:H8     | 1.72                     | 0.53              |
| 53:Ae:116:VAL:HG12 | 53:Ae:128:ALA:HB1  | 1.89                     | 0.53              |
| 59:Aj:82:ARG:NH1   | 59:Aj:133:GLN:OE1  | 2.37                     | 0.53              |
| 63:Ao:547:LEU:HG   | 63:Ao:550:ALA:HB3  | 1.90                     | 0.53              |
| 31:BA:562:A:H2'    | 31:BA:563:U:O4'    | 2.08                     | 0.53              |
| 31:BA:948:A:O2'    | 31:BA:1382:C:O2    | 2.21                     | 0.53              |
| 75:BC:704:ARG:HB3  | 75:BC:709:GLY:HA2  | 1.90                     | 0.53              |
| 2:BT:95:GLU:OE1    | 2:BT:145:LEU:N     | 2.36                     | 0.53              |
| 4:BV:160:VAL:HG22  | 4:BV:202:ILE:HG23  | 1.89                     | 0.53              |
| 31:AA:115:A:OP1    | 41:AO:203:ARG:NH2  | 2.41                     | 0.53              |
| 53:Ae:142:TRP:HZ2  | 59:Aj:76:LEU:HD11  | 1.73                     | 0.53              |
| 31:BA:220:G:N3     | 31:BA:231:C:O2'    | 2.42                     | 0.53              |
| 31:BA:978:G:H4'    | 31:BA:1429:C:H4'   | 1.90                     | 0.53              |
| 77:BE:195:ALA:H    | 77:BE:281:ASN:HD22 | 1.55                     | 0.53              |
| 2:BT:138:ILE:HD11  | 2:BT:152:ARG:HB2   | 1.90                     | 0.53              |
| 7:BY:47:GLU:OE1    | 7:BY:117:HIS:NE2   | 2.36                     | 0.53              |
| 31:AA:156:C:H2'    | 31:AA:157:A:C8     | 2.43                     | 0.53              |
| 31:AA:606:A:H3'    | 31:AA:607:G:H8     | 1.73                     | 0.53              |
| 63:Ao:465:PHE:HB3  | 63:Ao:495:THR:HG21 | 1.90                     | 0.53              |
| 75:BC:240:ALA:HB2  | 75:BC:243:ARG:HH21 | 1.72                     | 0.53              |
| 8:Ba:200:ARG:HD2   | 8:Ba:233:LYS:HD2   | 1.89                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 20:Bm:143:GLU:O    | 20:Bm:147:SER:OG   | 2.25                     | 0.53              |
| 22:Bo:45:GLU:OE2   | 22:Bo:70:ARG:NH2   | 2.40                     | 0.53              |
| 31:AA:13:U:H5''    | 34:AE:226:ARG:HH11 | 1.74                     | 0.53              |
| 59:Aj:88:GLN:O     | 64:Ap:215:ARG:NH1  | 2.41                     | 0.53              |
| 1:Al:340:ALA:N     | 31:AA:816:U:OP1    | 2.41                     | 0.53              |
| 33:AC:72:HIS:NE2   | 33:AC:75:ASN:OD1   | 2.41                     | 0.53              |
| 49:Aa:177:LYS:HB3  | 49:Aa:199:PRO:HD3  | 1.90                     | 0.53              |
| 31:BA:792:G:H2'    | 31:BA:793:A:H8     | 1.73                     | 0.53              |
| 31:BA:947:A:C2     | 83:BO:58:ILE:HG23  | 2.44                     | 0.53              |
| 7:BY:20:ARG:HG3    | 7:BY:41:ARG:HD3    | 1.90                     | 0.53              |
| 31:AA:201:A:H2'    | 31:AA:202:A:C8     | 2.44                     | 0.53              |
| 31:AA:759:U:H2'    | 31:AA:760:A:H8     | 1.73                     | 0.53              |
| 39:AL:63:LEU:HD11  | 39:AL:84:ARG:HB2   | 1.90                     | 0.53              |
| 31:BA:144:A:H2'    | 31:BA:145:A:C8     | 2.44                     | 0.53              |
| 31:BA:158:A:N3     | 31:BA:1039:A:O2'   | 2.33                     | 0.53              |
| 75:BC:327:ALA:HB2  | 75:BC:343:MET:HG2  | 1.91                     | 0.53              |
| 2:BT:91:LYS:HZ2    | 77:BE:105:GLY:HA3  | 1.74                     | 0.53              |
| 18:Bk:90:VAL:HG23  | 18:Bk:189:HIS:HB3  | 1.89                     | 0.53              |
| 31:AA:93:A:N3      | 52:Ad:79:ARG:NH2   | 2.57                     | 0.53              |
| 31:BA:1089:G:N1    | 31:BA:1125:U:O4    | 2.42                     | 0.53              |
| 75:BC:143:LEU:HD11 | 75:BC:155:THR:HG23 | 1.91                     | 0.53              |
| 25:Bt:9:ARG:NH2    | 31:BA:564:A:OP1    | 2.41                     | 0.53              |
| 31:AA:88:C:H2'     | 31:AA:89:U:C6      | 2.44                     | 0.53              |
| 31:AA:120:A:N6     | 31:AA:132:A:N1     | 2.57                     | 0.53              |
| 31:AA:420:A:N6     | 31:AA:441:U:OP2    | 2.39                     | 0.53              |
| 46:AV:70:C:H2'     | 46:AV:71:A:C4      | 2.42                     | 0.53              |
| 67:B3:105:SER:HB3  | 31:BA:416:U:H1'    | 1.91                     | 0.53              |
| 31:BA:119:A:C2     | 31:BA:129:A:N1     | 2.77                     | 0.53              |
| 31:BA:175:C:H5''   | 82:BN:115:ASN:HB2  | 1.91                     | 0.53              |
| 15:Bh:148:LEU:HD13 | 15:Bh:149:PRO:HD2  | 1.90                     | 0.53              |
| 31:AA:174:C:H1'    | 31:AA:207:G:H1'    | 1.91                     | 0.53              |
| 31:AA:524:U:H2'    | 31:AA:525:U:C6     | 2.43                     | 0.53              |
| 45:AU:30:LEU:HD22  | 45:AU:35:LEU:HD12  | 1.91                     | 0.53              |
| 31:BA:398:A:H3'    | 31:BA:399:A:H8     | 1.73                     | 0.53              |
| 31:BA:659:U:O2'    | 86:BR:82:GLU:OE2   | 2.27                     | 0.53              |
| 75:BC:579:PRO:HD3  | 75:BC:616:HIS:HD2  | 1.73                     | 0.53              |
| 81:BK:91:LEU:HD21  | 81:BK:144:ILE:HG23 | 1.91                     | 0.53              |
| 4:BV:102:VAL:HB    | 4:BV:139:LEU:HB3   | 1.92                     | 0.52              |
| 10:Bc:185:ARG:HG3  | 10:Bc:186:LEU:HD12 | 1.90                     | 0.52              |
| 18:Bk:122:GLU:N    | 18:Bk:158:GLN:O    | 2.42                     | 0.52              |
| 23:Bp:66:VAL:HG11  | 23:Bp:90:PHE:HE1   | 1.74                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:AA:302:U:OP1    | 41:AO:163:GLN:NE2  | 2.41                     | 0.52              |
| 49:Aa:192:ARG:O    | 49:Aa:211:ARG:NH1  | 2.39                     | 0.52              |
| 85:BQ:154:VAL:HG13 | 85:BQ:158:ARG:HD3  | 1.91                     | 0.52              |
| 31:AA:55:G:H2'     | 31:AA:56:U:C6      | 2.44                     | 0.52              |
| 31:AA:262:C:H2'    | 31:AA:263:G:H8     | 1.74                     | 0.52              |
| 53:Ae:188:MET:HB3  | 53:Ae:224:TYR:HE2  | 1.74                     | 0.52              |
| 69:B5:90:ASN:O     | 69:B5:94:ARG:HG2   | 2.09                     | 0.52              |
| 80:BJ:89:VAL:O     | 80:BJ:93:ASN:ND2   | 2.42                     | 0.52              |
| 82:BN:67:PHE:HD1   | 82:BN:71:LYS:HE2   | 1.74                     | 0.52              |
| 15:Bh:269:VAL:HG22 | 82:BN:11:TRP:HE1   | 1.74                     | 0.52              |
| 17:Bj:268:TYR:OH   | 74:BB:73:A:N3      | 2.43                     | 0.52              |
| 31:AA:226:G:H2'    | 31:AA:227:A:C8     | 2.45                     | 0.52              |
| 31:AA:552:A:O2'    | 31:AA:777:A:N3     | 2.40                     | 0.52              |
| 31:AA:597:U:O4     | 58:Ai:95:ARG:NH1   | 2.42                     | 0.52              |
| 31:AA:939:A:H2'    | 31:AA:940:C:H6     | 1.74                     | 0.52              |
| 36:AG:203:GLU:OE1  | 36:AG:207:GLN:NE2  | 2.42                     | 0.52              |
| 45:AU:82:ASP:OD1   | 45:AU:82:ASP:N     | 2.42                     | 0.52              |
| 49:Aa:338:GLU:HA   | 49:Aa:341:LYS:HG2  | 1.90                     | 0.52              |
| 53:Ae:162:GLN:OE1  | 53:Ae:196:ASN:ND2  | 2.33                     | 0.52              |
| 59:Aj:163:SER:HB3  | 59:Aj:190:MET:HB3  | 1.90                     | 0.52              |
| 72:B8:168:ARG:NE   | 31:BA:226:U:OP1    | 2.32                     | 0.52              |
| 31:BA:771:U:H2'    | 31:BA:772:G:H8     | 1.75                     | 0.52              |
| 31:BA:1026:A:O2'   | 31:BA:1277:G:N2    | 2.36                     | 0.52              |
| 31:BA:1079:U:H2'   | 31:BA:1080:A:H8    | 1.74                     | 0.52              |
| 31:BA:1145:C:N4    | 31:BA:1260:U:O4    | 2.42                     | 0.52              |
| 31:BA:1213:A:H2'   | 31:BA:1214:A:C8    | 2.43                     | 0.52              |
| 8:Ba:173:ARG:HE    | 8:Ba:303:ARG:HH21  | 1.56                     | 0.52              |
| 11:Bd:50:PHE:HE2   | 68:B4:50:ALA:HB2   | 1.74                     | 0.52              |
| 49:Aa:317:SER:HA   | 49:Aa:320:THR:HG22 | 1.92                     | 0.52              |
| 59:Aj:102:PRO:HB2  | 59:Aj:109:LEU:HD11 | 1.91                     | 0.52              |
| 59:Aj:107:GLU:OE1  | 59:Aj:108:ASN:N    | 2.41                     | 0.52              |
| 31:BA:301:U:H2'    | 31:BA:302:A:H8     | 1.73                     | 0.52              |
| 76:BD:141:ALA:HB2  | 76:BD:154:ALA:HB2  | 1.91                     | 0.52              |
| 80:BJ:162:LYS:H    | 80:BJ:162:LYS:HD2  | 1.75                     | 0.52              |
| 7:BY:145:ARG:HH22  | 7:BY:157:PRO:HD3   | 1.75                     | 0.52              |
| 9:Bb:240:ILE:HD13  | 9:Bb:248:GLY:HA3   | 1.92                     | 0.52              |
| 15:Bh:269:VAL:HG21 | 82:BN:15:ALA:HB1   | 1.92                     | 0.52              |
| 29:Bw:187:PRO:HD2  | 29:Bw:422:ARG:HH12 | 1.73                     | 0.52              |
| 31:AA:938:U:H2'    | 31:AA:939:A:C8     | 2.45                     | 0.52              |
| 56:Ag:129:LYS:HD2  | 56:Ag:319:ARG:HH21 | 1.75                     | 0.52              |
| 57:Ah:367:TRP:HA   | 57:Ah:370:ASN:HD21 | 1.73                     | 0.52              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 31:BA:317:A:H2'   | 31:BA:318:G:H8     | 1.73                     | 0.52              |
| 31:BA:784:G:O6    | 31:BA:1004:A:N6    | 2.42                     | 0.52              |
| 8:Ba:203:CYS:SG   | 8:Ba:205:GLN:NE2   | 2.82                     | 0.52              |
| 21:Bn:55:GLY:O    | 78:BF:249:ASN:ND2  | 2.42                     | 0.52              |
| 31:AA:29:A:O3'    | 39:AL:129:LYS:NZ   | 2.40                     | 0.52              |
| 56:Ag:198:LEU:O   | 56:Ag:222:GLY:N    | 2.43                     | 0.52              |
| 59:Aj:166:TYR:O   | 64:Ap:199:TRP:NE1  | 2.32                     | 0.52              |
| 60:Ak:239:GLU:OE1 | 60:Ak:241:TRP:NE1  | 2.35                     | 0.52              |
| 60:Ak:286:LEU:HA  | 60:Ak:291:VAL:HG21 | 1.91                     | 0.52              |
| 31:BA:505:U:C2    | 31:BA:507:G:H5'    | 2.44                     | 0.52              |
| 80:BJ:48:MET:SD   | 85:BQ:250:ARG:NH1  | 2.78                     | 0.52              |
| 80:BJ:95:MET:HE2  | 80:BJ:161:VAL:HG22 | 1.90                     | 0.52              |
| 8:Ba:244:GLU:O    | 8:Ba:248:THR:OG1   | 2.27                     | 0.52              |
| 23:Bp:35:GLN:OE1  | 80:BJ:150:HIS:ND1  | 2.42                     | 0.52              |
| 36:AG:130:SER:OG  | 36:AG:133:GLU:OE1  | 2.28                     | 0.52              |
| 42:AP:102:MET:SD  | 52:Ad:60:TYR:OH    | 2.62                     | 0.52              |
| 44:AR:130:TYR:OH  | 52:Ad:188:ASN:ND2  | 2.43                     | 0.52              |
| 63:Ao:363:MET:HE1 | 63:Ao:374:THR:HG21 | 1.91                     | 0.52              |
| 63:Ao:513:PRO:O   | 63:Ao:517:LYS:NZ   | 2.39                     | 0.52              |
| 65:CL:63:LYS:HG3  | 65:CL:66:GLN:HE21  | 1.74                     | 0.52              |
| 69:B5:84:ARG:NH2  | 31:BA:640:A:O2'    | 2.39                     | 0.52              |
| 31:BA:164:A:H4'   | 31:BA:165:A:C8     | 2.44                     | 0.52              |
| 31:BA:529:G:O2'   | 31:BA:548:A:N3     | 2.41                     | 0.52              |
| 31:BA:1416:G:H2'  | 31:BA:1417:A:H8    | 1.74                     | 0.52              |
| 75:BC:63:THR:HG23 | 75:BC:118:ILE:HD12 | 1.91                     | 0.52              |
| 31:AA:799:A:H2'   | 31:AA:800:G:C8     | 2.43                     | 0.52              |
| 56:Ag:383:SER:HB3 | 56:Ag:393:LEU:HD12 | 1.91                     | 0.52              |
| 67:B3:71:ARG:HA   | 67:B3:117:ILE:HG22 | 1.92                     | 0.52              |
| 69:B5:85:ARG:HH22 | 69:B5:93:ARG:HD3   | 1.75                     | 0.52              |
| 31:BA:378:U:OP1   | 84:BP:57:ARG:NE    | 2.41                     | 0.52              |
| 1:AI:358:THR:OG1  | 1:AI:359:GLU:N     | 2.43                     | 0.52              |
| 5:BW:153:ARG:NE   | 31:BA:687:U:OP1    | 2.42                     | 0.52              |
| 8:Ba:233:LYS:HA   | 8:Ba:286:PRO:HD2   | 1.91                     | 0.52              |
| 8:Ba:395:LYS:HD3  | 31:BA:269:U:H5''   | 1.91                     | 0.52              |
| 16:Bi:124:LYS:HE2 | 16:Bi:208:ILE:HD13 | 1.91                     | 0.52              |
| 28:B0:76:HIS:HD2  | 87:BS:70:THR:HG21  | 1.74                     | 0.52              |
| 31:AA:783:A:O2'   | 46:AY:37:C:O2      | 2.27                     | 0.52              |
| 31:AA:945:A:H5''  | 62:An:138:MET:HE1  | 1.92                     | 0.52              |
| 31:AA:948:U:H2'   | 31:AA:949:G:H8     | 1.73                     | 0.52              |
| 49:Aa:282:ASP:HA  | 49:Aa:285:ARG:HG2  | 1.92                     | 0.52              |
| 31:BA:740:U:H2'   | 31:BA:741:A:H8     | 1.73                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:BA:1279:G:H2'   | 31:BA:1280:C:H6    | 1.73                     | 0.52              |
| 31:BA:1569:A:O2'   | 31:BA:1570:C:O4'   | 2.19                     | 0.52              |
| 75:BC:520:LYS:NZ   | 75:BC:694:ASN:O    | 2.42                     | 0.52              |
| 86:BR:106:ARG:HD3  | 86:BR:136:LEU:HD11 | 1.91                     | 0.52              |
| 6:BX:35:GLN:HE21   | 6:BX:39:THR:HG21   | 1.75                     | 0.52              |
| 10:Bc:223:ALA:HB1  | 10:Bc:237:ILE:HD13 | 1.92                     | 0.52              |
| 31:AA:198:C:H2'    | 31:AA:199:G:C8     | 2.45                     | 0.52              |
| 31:AA:761:U:H2'    | 31:AA:762:G:C8     | 2.45                     | 0.52              |
| 34:AE:282:ILE:HG13 | 34:AE:327:ILE:HD13 | 1.92                     | 0.52              |
| 46:AV:23:A:H61     | 46:AV:41:A:H61     | 1.58                     | 0.52              |
| 67:B3:71:ARG:NH2   | 31:BA:473:G:OP2    | 2.42                     | 0.52              |
| 31:BA:990:U:H3'    | 31:BA:991:C:H2'    | 1.92                     | 0.52              |
| 85:BQ:124:VAL:HG12 | 85:BQ:158:ARG:HE   | 1.75                     | 0.52              |
| 8:Ba:108:HIS:HD2   | 8:Ba:110:ARG:H     | 1.56                     | 0.51              |
| 46:AY:4:A:H2'      | 46:AY:5:A:C8       | 2.45                     | 0.51              |
| 60:Ak:78:PHE:HE2   | 60:Ak:107:LEU:HD13 | 1.76                     | 0.51              |
| 8:Ba:41:PRO:HG2    | 31:BA:42:C:H41     | 1.75                     | 0.51              |
| 15:Bh:52:ARG:NH1   | 31:BA:148:A:OP1    | 2.43                     | 0.51              |
| 20:Bm:119:HIS:HB3  | 78:BF:62:VAL:HG23  | 1.91                     | 0.51              |
| 31:AA:578:G:H5''   | 31:AA:579:A:H2'    | 1.91                     | 0.51              |
| 37:AJ:124:VAL:O    | 40:AN:108:ARG:NH2  | 2.43                     | 0.51              |
| 38:AK:168:THR:HG21 | 45:AU:19:VAL:HG21  | 1.93                     | 0.51              |
| 56:Ag:49:ARG:HH11  | 56:Ag:68:ASN:HD21  | 1.58                     | 0.51              |
| 63:Ao:446:ASP:N    | 63:Ao:446:ASP:OD1  | 2.42                     | 0.51              |
| 86:BR:32:LEU:HB3   | 86:BR:52:LEU:HD22  | 1.92                     | 0.51              |
| 13:Bf:126:ARG:HH12 | 31:BA:173:C:H1'    | 1.74                     | 0.51              |
| 31:AA:491:G:H2'    | 31:AA:492:U:O4'    | 2.10                     | 0.51              |
| 49:Aa:189:HIS:O    | 49:Aa:211:ARG:NH2  | 2.43                     | 0.51              |
| 56:Ag:347:TYR:CZ   | 56:Ag:387:PRO:HB3  | 2.45                     | 0.51              |
| 74:BB:4:A:H3'      | 74:BB:5:A:H5''     | 1.93                     | 0.51              |
| 80:BJ:95:MET:HB3   | 80:BJ:156:SER:HB3  | 1.91                     | 0.51              |
| 7:BY:181:ASP:O     | 66:B2:95:LYS:NZ    | 2.32                     | 0.51              |
| 8:Ba:94:HIS:HA     | 8:Ba:99:TYR:CG     | 2.46                     | 0.51              |
| 15:Bh:60:ARG:HD2   | 15:Bh:63:LYS:HD2   | 1.93                     | 0.51              |
| 31:AA:25:U:H2'     | 31:AA:26:A:H8      | 1.74                     | 0.51              |
| 49:Aa:233:LYS:O    | 49:Aa:237:LEU:HB2  | 2.10                     | 0.51              |
| 53:Ae:69:LEU:HB3   | 53:Ae:405:LEU:HD23 | 1.92                     | 0.51              |
| 60:Ak:92:PRO:HB3   | 60:Ak:98:PRO:HD3   | 1.93                     | 0.51              |
| 72:B8:121:LEU:HD11 | 72:B8:183:ARG:HH21 | 1.75                     | 0.51              |
| 31:BA:671:C:H2'    | 31:BA:672:G:H8     | 1.75                     | 0.51              |
| 80:BJ:140:TYR:HB3  | 80:BJ:143:LEU:HD13 | 1.93                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 87:BS:122:VAL:HG22 | 87:BS:157:SER:HB3  | 1.92                     | 0.51              |
| 28:B0:85:LYS:NZ    | 31:BA:1207:C:OP1   | 2.35                     | 0.51              |
| 31:AA:315:U:OP1    | 31:AA:395:C:N4     | 2.44                     | 0.51              |
| 31:AA:631:A:N7     | 31:AA:654:A:N6     | 2.58                     | 0.51              |
| 33:AC:154:HIS:CG   | 60:Ak:77:PRO:HG3   | 2.46                     | 0.51              |
| 38:AK:83:GLU:OE1   | 38:AK:83:GLU:N     | 2.38                     | 0.51              |
| 49:Aa:154:LEU:HD12 | 49:Aa:260:ASP:HB3  | 1.92                     | 0.51              |
| 31:BA:889:C:H41    | 31:BA:1082:U:H4'   | 1.75                     | 0.51              |
| 31:BA:1021:C:H2'   | 31:BA:1022:G:C8    | 2.45                     | 0.51              |
| 31:BA:1042:A:O2'   | 31:BA:1561:A:N1    | 2.41                     | 0.51              |
| 74:BB:35:G:H2'     | 74:BB:36:A:H8      | 1.75                     | 0.51              |
| 75:BC:267:MET:HG3  | 75:BC:272:LYS:HD2  | 1.93                     | 0.51              |
| 75:BC:645:ILE:HD12 | 75:BC:728:GLN:HG3  | 1.92                     | 0.51              |
| 9:Bb:199:ALA:HA    | 9:Bb:256:PRO:HB3   | 1.91                     | 0.51              |
| 31:AA:356:A:H2'    | 31:AA:357:G:H8     | 1.75                     | 0.51              |
| 32:AB:221:ILE:HA   | 32:AB:235:VAL:HG23 | 1.92                     | 0.51              |
| 43:AQ:59:THR:OG1   | 43:AQ:60:VAL:N     | 2.43                     | 0.51              |
| 72:B8:133:LEU:N    | 31:BA:1244:U:OP1   | 2.42                     | 0.51              |
| 31:BA:942:U:H2'    | 31:BA:943:C:H6     | 1.76                     | 0.51              |
| 31:BA:1292:A:N6    | 31:BA:1304:G:O2'   | 2.44                     | 0.51              |
| 31:BA:1318:C:N4    | 31:BA:1319:G:O6    | 2.44                     | 0.51              |
| 76:BD:207:TYR:OH   | 76:BD:296:TYR:OH   | 2.26                     | 0.51              |
| 84:BP:168:GLU:OE1  | 84:BP:233:ARG:NH1  | 2.44                     | 0.51              |
| 84:BP:216:ASP:OD1  | 84:BP:217:ALA:N    | 2.44                     | 0.51              |
| 3:BU:114:LYS:NZ    | 13:Bf:45:CYS:O     | 2.38                     | 0.51              |
| 17:Bj:44:PRO:HG2   | 17:Bj:227:LEU:HA   | 1.93                     | 0.51              |
| 21:Bn:100:ASN:ND2  | 31:BA:68:A:N3      | 2.58                     | 0.51              |
| 29:Bw:308:GLN:HG2  | 31:BA:748:A:C8     | 2.45                     | 0.51              |
| 31:AA:765:A:N6     | 31:AA:805:G:C2     | 2.79                     | 0.51              |
| 31:AA:936:C:H2'    | 31:AA:937:A:C8     | 2.45                     | 0.51              |
| 34:AE:208:PRO:HB3  | 34:AE:214:THR:HG22 | 1.93                     | 0.51              |
| 36:AG:187:MET:HG2  | 36:AG:219:VAL:HG21 | 1.92                     | 0.51              |
| 38:AK:179:ASP:HB2  | 45:AU:26:LEU:HD21  | 1.93                     | 0.51              |
| 57:Ah:359:LYS:NZ   | 57:Ah:363:GLU:OE2  | 2.44                     | 0.51              |
| 71:B7:85:ARG:NH1   | 31:BA:125:A:OP1    | 2.44                     | 0.51              |
| 31:BA:361:C:OP2    | 84:BP:43:ARG:NH1   | 2.41                     | 0.51              |
| 31:BA:1521:U:H5    | 82:BN:177:ARG:HB3  | 1.75                     | 0.51              |
| 75:BC:537:PHE:HE2  | 75:BC:539:HIS:HB2  | 1.76                     | 0.51              |
| 75:BC:598:PRO:HG3  | 75:BC:638:LEU:HB3  | 1.92                     | 0.51              |
| 83:BO:100:PHE:HE2  | 83:BO:122:PRO:HG2  | 1.75                     | 0.51              |
| 87:BS:85:ARG:HG2   | 87:BS:90:ILE:HD12  | 1.92                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:BY:124:ASP:OD1   | 7:BY:124:ASP:N     | 2.44                     | 0.51              |
| 24:Bq:123:LYS:HG3  | 31:BA:531:G:H5''   | 1.91                     | 0.51              |
| 30:Bx:90:SER:HA    | 30:Bx:93:ILE:HD11  | 1.93                     | 0.51              |
| 31:AA:164:C:H3'    | 31:AA:165:G:H8     | 1.76                     | 0.51              |
| 31:AA:789:C:N3     | 31:AA:820:U:O2     | 2.44                     | 0.51              |
| 33:AC:113:ARG:HB2  | 37:AJ:166:GLU:HB3  | 1.92                     | 0.51              |
| 75:BC:176:LEU:HD11 | 75:BC:183:PRO:HG3  | 1.93                     | 0.51              |
| 82:BN:26:GLN:NE2   | 82:BN:147:GLN:OE1  | 2.43                     | 0.51              |
| 7:BY:121:LYS:HE3   | 7:BY:130:PRO:HB2   | 1.93                     | 0.51              |
| 32:AB:83:LEU:HD23  | 32:AB:247:LEU:HD21 | 1.93                     | 0.51              |
| 40:AN:93:MET:HG3   | 40:AN:110:VAL:HG11 | 1.93                     | 0.51              |
| 44:AR:66:CYS:HB3   | 44:AR:101:CYS:H    | 1.75                     | 0.51              |
| 54:B1:215:GLN:NE2  | 54:B1:219:GLU:OE2  | 2.33                     | 0.51              |
| 59:Aj:67:LEU:HB2   | 59:Aj:141:LEU:HD23 | 1.93                     | 0.51              |
| 63:Ao:541:ASP:OD1  | 63:Ao:542:GLN:N    | 2.40                     | 0.51              |
| 82:BN:104:VAL:HG13 | 82:BN:127:LEU:HD13 | 1.91                     | 0.51              |
| 83:BO:131:GLU:O    | 83:BO:135:SER:OG   | 2.27                     | 0.51              |
| 8:Ba:351:LEU:HD11  | 8:Ba:379:ASP:HA    | 1.92                     | 0.51              |
| 9:Bb:330:VAL:HG13  | 9:Bb:334:LEU:HD12  | 1.93                     | 0.51              |
| 15:Bh:264:THR:OG1  | 82:BN:136:ASP:O    | 2.28                     | 0.51              |
| 30:Bx:133:PRO:HD3  | 31:BA:1529:A:H2    | 1.76                     | 0.51              |
| 31:AA:786:U:H2'    | 31:AA:787:A:C8     | 2.46                     | 0.51              |
| 34:AE:282:ILE:HD12 | 34:AE:353:LEU:HB3  | 1.93                     | 0.51              |
| 34:AE:296:LEU:HD22 | 34:AE:352:GLY:HA3  | 1.92                     | 0.51              |
| 49:Aa:167:ASP:OD2  | 49:Aa:197:ARG:NH1  | 2.43                     | 0.51              |
| 31:BA:445:A:H2     | 85:BQ:244:LYS:HD3  | 1.75                     | 0.51              |
| 31:BA:1042:A:H2'   | 31:BA:1043:A:H8    | 1.76                     | 0.51              |
| 85:BQ:89:ILE:HD11  | 85:BQ:176:LEU:HD22 | 1.93                     | 0.51              |
| 85:BQ:172:VAL:HA   | 85:BQ:175:PHE:HD1  | 1.76                     | 0.51              |
| 37:AJ:163:ASN:HB3  | 60:Ak:116:LEU:HD11 | 1.94                     | 0.50              |
| 65:LL:135:THR:HG22 | 65:LL:136:GLU:HG3  | 1.92                     | 0.50              |
| 31:BA:947:A:H2     | 83:BO:58:ILE:HG23  | 1.76                     | 0.50              |
| 78:BF:55:VAL:HA    | 78:BF:83:HIS:HE1   | 1.77                     | 0.50              |
| 8:Ba:140:ALA:HB1   | 8:Ba:412:ARG:HG2   | 1.92                     | 0.50              |
| 14:Bg:27:GLN:HB2   | 14:Bg:80:LEU:HD12  | 1.93                     | 0.50              |
| 15:Bh:302:ARG:NH2  | 82:BN:3:SER:O      | 2.36                     | 0.50              |
| 31:AA:526:G:H2'    | 31:AA:527:G:C8     | 2.46                     | 0.50              |
| 34:AE:180:ASP:OD1  | 34:AE:180:ASP:N    | 2.44                     | 0.50              |
| 53:Ae:213:PHE:HE2  | 53:Ae:221:LEU:HD12 | 1.76                     | 0.50              |
| 67:B3:77:ARG:NH1   | 31:BA:469:C:OP2    | 2.38                     | 0.50              |
| 31:BA:183:U:H2'    | 31:BA:184:U:C6     | 2.46                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:BA:942:U:H2'    | 31:BA:943:C:C6     | 2.45                     | 0.50              |
| 76:BD:219:ARG:HE   | 76:BD:226:ILE:HD12 | 1.77                     | 0.50              |
| 8:Ba:343:GLN:HG2   | 8:Ba:356:VAL:HG22  | 1.94                     | 0.50              |
| 14:Bg:19:LEU:HD23  | 15:Bh:221:THR:HG22 | 1.93                     | 0.50              |
| 16:Bi:190:GLU:OE1  | 16:Bi:215:ARG:NH2  | 2.44                     | 0.50              |
| 22:Bo:75:ARG:HE    | 67:B3:134:MET:HG3  | 1.76                     | 0.50              |
| 68:B4:71:GLU:O     | 68:B4:73:ARG:N     | 2.43                     | 0.50              |
| 31:BA:229:A:H4'    | 31:BA:230:G:H5'    | 1.92                     | 0.50              |
| 31:BA:312:C:H2'    | 31:BA:313:U:C6     | 2.46                     | 0.50              |
| 31:BA:1459:U:C2    | 31:BA:1468:A:N7    | 2.80                     | 0.50              |
| 31:BA:1519:U:OP2   | 31:BA:1520:U:O2'   | 2.21                     | 0.50              |
| 7:BY:40:ARG:HD3    | 31:BA:115:U:C4     | 2.46                     | 0.50              |
| 31:AA:154:C:H2'    | 31:AA:155:A:C8     | 2.46                     | 0.50              |
| 31:AA:378:A:H2'    | 31:AA:379:A:H8     | 1.76                     | 0.50              |
| 31:AA:386:U:H4'    | 35:AF:94:VAL:HG12  | 1.93                     | 0.50              |
| 31:AA:822:A:H3'    | 31:AA:823:G:H8     | 1.75                     | 0.50              |
| 52:Ad:94:LYS:HA    | 52:Ad:97:GLU:HG2   | 1.92                     | 0.50              |
| 59:Aj:98:THR:HG22  | 59:Aj:116:GLY:HA2  | 1.94                     | 0.50              |
| 63:Ao:137:ILE:HD12 | 63:Ao:138:PRO:HD2  | 1.92                     | 0.50              |
| 63:Ao:259:ALA:HA   | 63:Ao:262:TYR:CZ   | 2.46                     | 0.50              |
| 63:Ao:432:LEU:HD13 | 63:Ao:471:MET:HB3  | 1.93                     | 0.50              |
| 63:Ao:474:ILE:HG21 | 63:Ao:508:ARG:HG3  | 1.92                     | 0.50              |
| 31:BA:983:U:O4     | 31:BA:984:A:N6     | 2.45                     | 0.50              |
| 31:BA:1399:G:O2'   | 31:BA:1402:C:OP2   | 2.19                     | 0.50              |
| 31:BA:1414:C:H2'   | 31:BA:1415:G:C8    | 2.46                     | 0.50              |
| 9:Bb:124:ARG:HH21  | 11:Bd:75:LYS:HD2   | 1.76                     | 0.50              |
| 31:AA:189:A:H2'    | 31:AA:190:G:C8     | 2.47                     | 0.50              |
| 31:AA:641:A:N7     | 34:AE:260:LYS:NZ   | 2.59                     | 0.50              |
| 36:AG:61:GLU:HA    | 36:AG:64:TYR:HD1   | 1.75                     | 0.50              |
| 42:AP:102:MET:O    | 42:AP:106:ASN:ND2  | 2.30                     | 0.50              |
| 44:AR:53:VAL:HG11  | 50:Ab:66:HIS:HE1   | 1.77                     | 0.50              |
| 64:Ap:89:ARG:HD3   | 64:Ap:144:MET:HE3  | 1.93                     | 0.50              |
| 65:CL:71:ILE:HG12  | 65:DL:67:LEU:HD11  | 1.94                     | 0.50              |
| 31:BA:299:A:OP2    | 31:BA:833:C:N4     | 2.45                     | 0.50              |
| 31:BA:1072:A:H2'   | 31:BA:1073:A:C8    | 2.46                     | 0.50              |
| 31:BA:1076:A:N6    | 31:BA:1140:A:O2'   | 2.44                     | 0.50              |
| 31:BA:1506:A:H2'   | 31:BA:1507:G:C8    | 2.47                     | 0.50              |
| 3:BU:33:GLY:O      | 3:BU:36:ASN:ND2    | 2.45                     | 0.50              |
| 4:BV:138:LEU:HD21  | 22:Bo:43:LEU:HD11  | 1.94                     | 0.50              |
| 9:Bb:226:LEU:HD21  | 87:BS:43:ALA:HB1   | 1.92                     | 0.50              |
| 14:Bg:15:LEU:HD11  | 15:Bh:169:VAL:HG22 | 1.93                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 17:Bj:162:ARG:HH21 | 17:Bj:164:LYS:HE2  | 1.76                     | 0.50              |
| 30:Bx:182:LYS:NZ   | 31:BA:491:U:OP1    | 2.35                     | 0.50              |
| 36:AG:176:ASP:HA   | 36:AG:179:ARG:HE   | 1.76                     | 0.50              |
| 56:Ag:154:ILE:HD13 | 56:Ag:261:VAL:HB   | 1.92                     | 0.50              |
| 58:Ai:53:PRO:HB2   | 58:Ai:58:TYR:HE2   | 1.76                     | 0.50              |
| 31:BA:130:A:H2'    | 31:BA:131:A:O4'    | 2.12                     | 0.50              |
| 31:BA:1528:A:H2'   | 31:BA:1529:A:H8    | 1.76                     | 0.50              |
| 75:BC:557:GLU:OE1  | 75:BC:557:GLU:N    | 2.45                     | 0.50              |
| 10:Bc:206:LEU:HD12 | 10:Bc:209:LYS:HE3  | 1.94                     | 0.50              |
| 15:Bh:128:GLN:OE1  | 15:Bh:204:GLN:NE2  | 2.41                     | 0.50              |
| 16:Bi:192:PRO:HB3  | 16:Bi:216:MET:HG2  | 1.94                     | 0.50              |
| 17:Bj:245:GLN:HG3  | 17:Bj:248:LYS:HB3  | 1.93                     | 0.50              |
| 31:AA:913:G:H2'    | 31:AA:914:A:C8     | 2.45                     | 0.50              |
| 39:AL:102:LEU:HD21 | 39:AL:132:CYS:HB2  | 1.93                     | 0.50              |
| 54:B1:140:GLY:HA3  | 54:B1:143:PHE:HD2  | 1.77                     | 0.50              |
| 71:B7:91:LYS:N     | 31:BA:118:U:OP1    | 2.45                     | 0.50              |
| 31:BA:49:A:H2'     | 31:BA:50:A:C8      | 2.47                     | 0.50              |
| 31:BA:619:C:H2'    | 31:BA:620:A:C8     | 2.47                     | 0.50              |
| 31:BA:916:C:H2'    | 31:BA:917:G:C8     | 2.46                     | 0.50              |
| 1:AI:139:GLN:HB2   | 1:AI:140:TRP:CE3   | 2.46                     | 0.50              |
| 20:Bm:89:ASP:OD1   | 20:Bm:125:ARG:NH2  | 2.40                     | 0.50              |
| 29:Bw:369:ASN:H    | 29:Bw:385:ASN:HD22 | 1.57                     | 0.50              |
| 31:AA:876:A:H5'    | 31:AA:877:A:H5'    | 1.94                     | 0.50              |
| 56:Ag:160:TRP:HB3  | 56:Ag:179:GLN:HE22 | 1.77                     | 0.50              |
| 65:FL:83:ASN:ND2   | 80:BJ:218:THR:OG1  | 2.45                     | 0.50              |
| 68:B4:53:TYR:CG    | 68:B4:72:PRO:HB3   | 2.47                     | 0.50              |
| 31:BA:477:A:N6     | 31:BA:478:G:O6     | 2.44                     | 0.50              |
| 75:BC:530:THR:OG1  | 75:BC:642:THR:OG1  | 2.26                     | 0.50              |
| 78:BF:171:VAL:HG13 | 78:BF:273:LEU:HD22 | 1.94                     | 0.50              |
| 80:BJ:181:ILE:O    | 80:BJ:184:THR:OG1  | 2.25                     | 0.50              |
| 31:AA:14:C:OP1     | 34:AE:341:ASN:ND2  | 2.45                     | 0.50              |
| 42:AP:64:LYS:HE3   | 49:Aa:176:ALA:HB3  | 1.92                     | 0.50              |
| 31:BA:83:A:OP2     | 31:BA:1235:C:O2'   | 2.19                     | 0.50              |
| 31:BA:289:U:H2'    | 31:BA:290:A:C8     | 2.45                     | 0.50              |
| 31:BA:548:A:H2'    | 31:BA:549:C:C6     | 2.47                     | 0.50              |
| 31:BA:1479:G:H2'   | 31:BA:1480:G:H8    | 1.77                     | 0.50              |
| 76:BD:133:ASP:OD2  | 76:BD:136:ARG:NH1  | 2.45                     | 0.50              |
| 1:AI:257:LEU:HD23  | 1:AI:257:LEU:H     | 1.77                     | 0.49              |
| 31:AA:356:A:H2'    | 31:AA:357:G:C8     | 2.47                     | 0.49              |
| 36:AG:57:GLU:OE1   | 36:AG:57:GLU:N     | 2.45                     | 0.49              |
| 53:Ae:108:SER:O    | 53:Ae:111:THR:OG1  | 2.29                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 60:Ak:60:GLU:OE1   | 60:Ak:60:GLU:N     | 2.44                     | 0.49              |
| 68:B4:59:LYS:HA    | 68:B4:78:MET:HB2   | 1.93                     | 0.49              |
| 5:BW:48:LYS:N      | 31:BA:2:C:OP1      | 2.43                     | 0.49              |
| 18:Bk:49:ARG:NH2   | 31:BA:407:A:OP2    | 2.27                     | 0.49              |
| 31:AA:57:A:O2'     | 31:AA:59:C:OP1     | 2.23                     | 0.49              |
| 31:AA:869:A:N6     | 31:AA:899:C:O2'    | 2.45                     | 0.49              |
| 39:AL:109:LEU:HB2  | 39:AL:129:LYS:HG2  | 1.93                     | 0.49              |
| 63:Ao:541:ASP:OD1  | 63:Ao:542:GLN:NE2  | 2.45                     | 0.49              |
| 31:BA:411:U:H2'    | 31:BA:412:C:C6     | 2.47                     | 0.49              |
| 31:BA:922:A:O2'    | 31:BA:923:A:O4'    | 2.29                     | 0.49              |
| 3:BU:52:LYS:NZ     | 31:BA:164:A:OP1    | 2.42                     | 0.49              |
| 19:Bl:144:THR:OG1  | 78:BF:92:ARG:NH2   | 2.45                     | 0.49              |
| 26:Bu:138:CYS:SG   | 26:Bu:139:SER:N    | 2.86                     | 0.49              |
| 31:AA:489:G:H2'    | 31:AA:490:A:H8     | 1.77                     | 0.49              |
| 42:AP:51:LEU:HD13  | 42:AP:73:ILE:HG12  | 1.95                     | 0.49              |
| 53:Ae:392:SER:HB2  | 53:Ae:395:THR:HG22 | 1.93                     | 0.49              |
| 56:Ag:104:ALA:HB1  | 56:Ag:139:HIS:HD2  | 1.77                     | 0.49              |
| 57:Ah:311:ALA:O    | 60:Ak:166:ARG:NH2  | 2.37                     | 0.49              |
| 58:Ai:19:PHE:O     | 60:Ak:213:ARG:NH1  | 2.46                     | 0.49              |
| 59:Aj:41:MET:HE3   | 59:Aj:50:LEU:HD12  | 1.94                     | 0.49              |
| 69:B5:93:ARG:NH1   | 31:BA:644:G:OP1    | 2.33                     | 0.49              |
| 75:BC:187:LEU:HB2  | 75:BC:200:PHE:HE1  | 1.78                     | 0.49              |
| 81:BK:26:ALA:HB3   | 81:BK:62:GLU:HA    | 1.93                     | 0.49              |
| 5:BW:147:ARG:HH12  | 31:BA:639:U:H5'    | 1.77                     | 0.49              |
| 5:BW:154:ILE:HG13  | 16:Bi:52:SER:HB3   | 1.94                     | 0.49              |
| 5:BW:189:THR:HG23  | 5:BW:192:ALA:H     | 1.78                     | 0.49              |
| 19:Bl:96:VAL:HG22  | 19:Bl:110:ILE:HG12 | 1.94                     | 0.49              |
| 31:AA:476:A:H8     | 61:Am:13:LEU:HD22  | 1.76                     | 0.49              |
| 31:AA:893:A:H2'    | 31:AA:894:U:O4'    | 2.12                     | 0.49              |
| 31:BA:329:A:C5     | 76:BD:275:LEU:HB2  | 2.47                     | 0.49              |
| 75:BC:579:PRO:HD3  | 75:BC:616:HIS:CD2  | 2.47                     | 0.49              |
| 87:BS:114:LYS:HE3  | 87:BS:115:HIS:CE1  | 2.47                     | 0.49              |
| 1:AI:273:GLY:HA3   | 1:AI:352:ALA:HB2   | 1.94                     | 0.49              |
| 4:BV:139:LEU:HD11  | 4:BV:146:THR:HG23  | 1.93                     | 0.49              |
| 9:Bb:155:CYS:O     | 9:Bb:267:ARG:NH1   | 2.46                     | 0.49              |
| 11:Bd:23:ARG:HH11  | 46:AV:43:A:H4'     | 1.77                     | 0.49              |
| 29:Bw:240:GLN:NE2  | 29:Bw:348:PRO:O    | 2.46                     | 0.49              |
| 31:AA:189:A:H2'    | 31:AA:190:G:H8     | 1.77                     | 0.49              |
| 34:AE:203:LEU:HD21 | 34:AE:268:PHE:HB3  | 1.94                     | 0.49              |
| 34:AE:313:GLY:HA2  | 34:AE:331:ASP:HA   | 1.93                     | 0.49              |
| 41:AO:176:TYR:HB2  | 43:AQ:89:GLY:HA3   | 1.94                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:BA:335:U:OP1    | 31:BA:338:C:N4     | 2.34                     | 0.49              |
| 31:BA:343:C:H2'    | 31:BA:344:U:C6     | 2.47                     | 0.49              |
| 31:BA:799:A:H61    | 31:BA:991:C:H42    | 1.60                     | 0.49              |
| 31:BA:1497:G:H1'   | 31:BA:1498:C:H2'   | 1.93                     | 0.49              |
| 5:BW:101:LEU:HD22  | 5:BW:116:LYS:HG3   | 1.94                     | 0.49              |
| 9:Bb:257:PRO:HB3   | 9:Bb:268:PHE:CZ    | 2.48                     | 0.49              |
| 10:Bc:52:GLN:HG3   | 10:Bc:216:LEU:HD11 | 1.94                     | 0.49              |
| 30:Bx:188:SER:HB3  | 31:BA:576:U:H5''   | 1.93                     | 0.49              |
| 31:AA:158:C:O3'    | 31:AA:172:A:N6     | 2.46                     | 0.49              |
| 31:AA:279:U:O2'    | 39:AL:54:GLY:O     | 2.30                     | 0.49              |
| 34:AE:93:LEU:H     | 58:Ai:75:HIS:HD2   | 1.60                     | 0.49              |
| 46:AV:3:U:O4       | 46:AV:4:A:N6       | 2.46                     | 0.49              |
| 59:Aj:206:LYS:NZ   | 59:Aj:208:GLU:O    | 2.46                     | 0.49              |
| 31:BA:218:A:N6     | 31:BA:229:A:O4'    | 2.46                     | 0.49              |
| 31:BA:898:C:H5'    | 76:BD:279:LYS:HB2  | 1.95                     | 0.49              |
| 1:AI:148:HIS:CE1   | 1:AI:160:SER:HB3   | 2.48                     | 0.49              |
| 4:BV:71:PRO:HB2    | 4:BV:76:GLU:HG2    | 1.93                     | 0.49              |
| 8:Ba:207:ASN:HB3   | 29:Bw:151:LEU:HD11 | 1.95                     | 0.49              |
| 17:Bj:260:LEU:HD22 | 17:Bj:273:ARG:HD2  | 1.93                     | 0.49              |
| 25:Bt:35:MET:HE3   | 80:BJ:46:LYS:HE2   | 1.95                     | 0.49              |
| 31:AA:831:A:H2'    | 31:AA:832:G:C8     | 2.48                     | 0.49              |
| 34:AE:203:LEU:HD22 | 34:AE:222:ILE:HD11 | 1.95                     | 0.49              |
| 44:AR:49:GLU:OE1   | 44:AR:49:GLU:N     | 2.38                     | 0.49              |
| 31:BA:247:C:H2'    | 31:BA:248:A:H8     | 1.77                     | 0.49              |
| 31:BA:368:A:H62    | 31:BA:433:G:H5'    | 1.77                     | 0.49              |
| 31:BA:672:G:H21    | 31:BA:759:C:H5'    | 1.77                     | 0.49              |
| 76:BD:216:VAL:HG13 | 76:BD:228:GLN:HB3  | 1.94                     | 0.49              |
| 81:BK:101:ALA:HB2  | 81:BK:109:ALA:HB2  | 1.95                     | 0.49              |
| 1:AI:338:ARG:HH11  | 31:AA:816:U:H4'    | 1.78                     | 0.49              |
| 19:Bl:96:VAL:O     | 19:Bl:158:LYS:NZ   | 2.40                     | 0.49              |
| 31:AA:534:U:H2'    | 31:AA:535:U:C6     | 2.48                     | 0.49              |
| 45:AU:72:ILE:HD12  | 61:Am:104:LEU:HD22 | 1.95                     | 0.49              |
| 49:Aa:185:TYR:HB2  | 51:Ac:125:HIS:CE1  | 2.48                     | 0.49              |
| 49:Aa:348:HIS:CD2  | 49:Aa:351:LYS:HB2  | 2.47                     | 0.49              |
| 58:Ai:55:HIS:HA    | 58:Ai:58:TYR:HD2   | 1.77                     | 0.49              |
| 60:Ak:67:ASP:N     | 60:Ak:67:ASP:OD1   | 2.42                     | 0.49              |
| 31:BA:311:A:H5'    | 76:BD:262:GLY:HA2  | 1.94                     | 0.49              |
| 31:BA:504:G:H2'    | 31:BA:505:U:C5     | 2.48                     | 0.49              |
| 31:BA:974:C:H2'    | 31:BA:975:G:C8     | 2.48                     | 0.49              |
| 75:BC:53:ALA:N     | 75:BC:59:LYS:HD3   | 2.27                     | 0.49              |
| 15:Bh:263:SER:H    | 82:BN:140:ASN:HD22 | 1.60                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 28:B0:102:GLU:OE2  | 28:B0:132:HIS:NE2  | 2.26                     | 0.49              |
| 29:Bw:60:GLN:NE2   | 29:Bw:376:GLN:OE1  | 2.37                     | 0.49              |
| 31:AA:546:U:H2'    | 31:AA:547:A:C8     | 2.47                     | 0.49              |
| 35:AF:6:LEU:HB3    | 35:AF:66:VAL:HB    | 1.94                     | 0.49              |
| 43:AQ:63:ILE:HG22  | 43:AQ:85:ILE:HD12  | 1.95                     | 0.49              |
| 73:B9:69:LEU:HD22  | 73:B9:97:GLN:HB3   | 1.94                     | 0.49              |
| 31:BA:476:U:H2'    | 31:BA:477:A:H8     | 1.78                     | 0.49              |
| 31:BA:1402:C:O2'   | 77:BE:233:GLN:OE1  | 2.21                     | 0.49              |
| 80:BJ:157:GLU:HG3  | 80:BJ:158:GLU:HG2  | 1.95                     | 0.49              |
| 9:Bb:191:ASN:O     | 9:Bb:320:GLN:N     | 2.36                     | 0.49              |
| 27:Bv:33:ARG:HH12  | 78:BF:287:ARG:HD2  | 1.76                     | 0.49              |
| 29:Bw:93:VAL:HB    | 29:Bw:227:ILE:HG12 | 1.95                     | 0.49              |
| 31:AA:70:U:H2'     | 31:AA:71:G:C8      | 2.47                     | 0.49              |
| 31:AA:85:G:H2'     | 31:AA:86:A:H8      | 1.77                     | 0.49              |
| 31:AA:121:C:O2'    | 43:AQ:23:GLN:O     | 2.30                     | 0.49              |
| 31:AA:378:A:H2'    | 31:AA:379:A:C8     | 2.47                     | 0.49              |
| 31:AA:591:A:H2'    | 31:AA:592:A:H8     | 1.78                     | 0.49              |
| 32:AB:79:SER:N     | 32:AB:82:SER:OG    | 2.36                     | 0.49              |
| 37:AJ:125:HIS:CD2  | 37:AJ:126:ILE:HG12 | 2.48                     | 0.49              |
| 57:Ah:350:LEU:HD22 | 57:Ah:361:LYS:HG2  | 1.95                     | 0.49              |
| 65:EL:72:ALA:HA    | 65:HL:76:LEU:HB2   | 1.94                     | 0.49              |
| 67:B3:78:ARG:HH12  | 85:BQ:225:GLY:HA3  | 1.78                     | 0.49              |
| 31:BA:266:C:O2'    | 31:BA:281:A:N6     | 2.38                     | 0.49              |
| 74:BB:40:U:H2'     | 74:BB:41:G:H8      | 1.76                     | 0.49              |
| 76:BD:290:LEU:HD12 | 76:BD:291:PRO:HD2  | 1.95                     | 0.49              |
| 77:BE:94:SER:HA    | 77:BE:182:THR:HG21 | 1.94                     | 0.49              |
| 84:BP:153:ASN:HD22 | 84:BP:173:VAL:HB   | 1.76                     | 0.49              |
| 3:BU:95:VAL:HG12   | 3:BU:97:LEU:HG     | 1.95                     | 0.48              |
| 8:Ba:380:GLN:HB3   | 8:Ba:410:THR:HG22  | 1.95                     | 0.48              |
| 10:Bc:190:MET:HG2  | 10:Bc:291:ARG:HH12 | 1.77                     | 0.48              |
| 31:AA:561:U:H3'    | 31:AA:562:A:C2     | 2.47                     | 0.48              |
| 31:AA:620:C:OP2    | 33:AC:38:ARG:N     | 2.39                     | 0.48              |
| 36:AG:139:ARG:NH2  | 56:Ag:366:GLN:HE22 | 2.11                     | 0.48              |
| 43:AQ:50:PHE:HD2   | 43:AQ:76:HIS:HB3   | 1.77                     | 0.48              |
| 65:FL:66:GLN:HG2   | 65:FL:67:LEU:HD22  | 1.95                     | 0.48              |
| 31:BA:53:U:H2'     | 31:BA:54:A:H8      | 1.78                     | 0.48              |
| 31:BA:164:A:N1     | 31:BA:1030:G:N2    | 2.61                     | 0.48              |
| 31:BA:481:A:H2'    | 31:BA:482:G:C8     | 2.48                     | 0.48              |
| 31:BA:1279:G:H2'   | 31:BA:1280:C:C6    | 2.47                     | 0.48              |
| 85:BQ:96:TYR:OH    | 85:BQ:129:LYS:NZ   | 2.32                     | 0.48              |
| 2:BT:251:GLU:HG2   | 2:BT:255:ARG:HH11  | 1.76                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 6:BX:145:PRO:HG3   | 16:Bi:176:ILE:HD13 | 1.94                     | 0.48              |
| 11:Bd:23:ARG:O     | 11:Bd:27:ARG:HG2   | 2.13                     | 0.48              |
| 11:Bd:25:LYS:O     | 11:Bd:29:ARG:HD3   | 2.13                     | 0.48              |
| 31:AA:159:C:P      | 31:AA:172:A:H61    | 2.35                     | 0.48              |
| 43:AQ:50:PHE:HB3   | 43:AQ:77:VAL:HG22  | 1.95                     | 0.48              |
| 46:AY:11:G:H2'     | 46:AY:12:C:C6      | 2.48                     | 0.48              |
| 51:Ac:76:LEU:HD22  | 51:Ac:102:ILE:HD11 | 1.94                     | 0.48              |
| 31:BA:243:A:O5'    | 78:BF:126:LYS:NZ   | 2.46                     | 0.48              |
| 31:BA:1003:C:H2'   | 31:BA:1004:A:H8    | 1.78                     | 0.48              |
| 31:BA:1020:C:H2'   | 31:BA:1021:C:C6    | 2.48                     | 0.48              |
| 83:BO:77:ILE:HG22  | 83:BO:78:ARG:HG3   | 1.95                     | 0.48              |
| 84:BP:226:PRO:HA   | 84:BP:229:PHE:CD1  | 2.48                     | 0.48              |
| 5:BW:154:ILE:HG12  | 16:Bi:47:GLN:HE21  | 1.78                     | 0.48              |
| 31:AA:54:A:OP2     | 52:Ad:27:ARG:NH1   | 2.46                     | 0.48              |
| 31:AA:308:A:H3'    | 31:AA:309:A:H5'    | 1.95                     | 0.48              |
| 32:AB:99:ARG:NH1   | 50:Ab:50:ARG:O     | 2.41                     | 0.48              |
| 33:AC:72:HIS:HB3   | 33:AC:112:ARG:HH11 | 1.79                     | 0.48              |
| 40:AN:80:ARG:HG3   | 40:AN:86:ARG:HD2   | 1.94                     | 0.48              |
| 49:Aa:135:GLU:HA   | 49:Aa:138:LYS:HG2  | 1.94                     | 0.48              |
| 63:Ao:427:SER:HA   | 63:Ao:467:LEU:HD11 | 1.95                     | 0.48              |
| 63:Ao:485:ILE:HG23 | 63:Ao:491:PRO:HD3  | 1.95                     | 0.48              |
| 80:BJ:119:HIS:CE1  | 80:BJ:160:LYS:HB2  | 2.48                     | 0.48              |
| 3:BU:92:LYS:HZ2    | 22:Bo:27:TRP:CD1   | 2.31                     | 0.48              |
| 8:Ba:309:LEU:HG    | 8:Ba:313:MET:HE3   | 1.95                     | 0.48              |
| 25:Bt:81:ARG:HH12  | 31:BA:388:A:H3'    | 1.79                     | 0.48              |
| 28:B0:49:LYS:HZ1   | 31:BA:1161:G:H5''  | 1.78                     | 0.48              |
| 31:AA:789:C:O2     | 31:AA:820:U:N3     | 2.45                     | 0.48              |
| 39:AL:99:GLY:O     | 39:AL:127:ARG:NH2  | 2.38                     | 0.48              |
| 31:BA:274:A:O4'    | 31:BA:309:A:O2'    | 2.31                     | 0.48              |
| 31:BA:869:G:H2'    | 31:BA:870:C:C6     | 2.48                     | 0.48              |
| 74:BB:31:C:H2'     | 74:BB:32:A:H8      | 1.79                     | 0.48              |
| 75:BC:593:ALA:HB2  | 75:BC:631:GLU:HG2  | 1.94                     | 0.48              |
| 9:Bb:110:LEU:HD11  | 87:BS:113:LYS:HE2  | 1.94                     | 0.48              |
| 15:Bh:69:HIS:HE1   | 15:Bh:85:LEU:HD13  | 1.77                     | 0.48              |
| 27:Bv:28:ARG:NH1   | 31:BA:100:C:HO2'   | 2.11                     | 0.48              |
| 31:AA:96:U:H2'     | 31:AA:97:C:C6      | 2.48                     | 0.48              |
| 31:AA:217:U:H2'    | 31:AA:218:A:H8     | 1.78                     | 0.48              |
| 31:AA:299:U:H2'    | 31:AA:300:G:H8     | 1.78                     | 0.48              |
| 34:AE:305:MET:HE3  | 34:AE:332:LEU:HD21 | 1.96                     | 0.48              |
| 36:AG:241:TRP:CD1  | 61:Am:40:LYS:HZ2   | 2.31                     | 0.48              |
| 39:AL:96:PRO:O     | 39:AL:127:ARG:NH1  | 2.45                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 46:AY:15:A:O2'     | 46:AY:16:A:H5''    | 2.12                     | 0.48              |
| 58:Ai:75:HIS:CE1   | 58:Ai:79:ARG:HE    | 2.32                     | 0.48              |
| 65:GL:68:VAL:HG21  | 65:HL:85:LEU:HD23  | 1.95                     | 0.48              |
| 69:B5:141:MET:HB2  | 69:B5:173:ARG:HH12 | 1.78                     | 0.48              |
| 31:BA:799:A:H61    | 31:BA:991:C:N4     | 2.11                     | 0.48              |
| 31:BA:1222:A:H2'   | 31:BA:1223:U:C6    | 2.49                     | 0.48              |
| 74:BB:43:C:H2'     | 74:BB:44:U:H5'     | 1.94                     | 0.48              |
| 76:BD:218:LEU:HD11 | 76:BD:228:GLN:HB2  | 1.94                     | 0.48              |
| 5:BW:160:GLY:HA3   | 16:Bi:44:PRO:HG3   | 1.96                     | 0.48              |
| 9:Bb:233:VAL:O     | 9:Bb:296:ARG:NH1   | 2.45                     | 0.48              |
| 11:Bd:66:GLU:HA    | 11:Bd:69:ARG:HG2   | 1.94                     | 0.48              |
| 20:Bm:117:ARG:O    | 20:Bm:121:MET:HG2  | 2.13                     | 0.48              |
| 30:Bx:79:HIS:NE2   | 30:Bx:183:ASP:OD2  | 2.46                     | 0.48              |
| 31:AA:97:C:H2'     | 31:AA:98:A:O4'     | 2.14                     | 0.48              |
| 58:Ai:46:LYS:HA    | 58:Ai:49:TYR:CD2   | 2.49                     | 0.48              |
| 63:Ao:537:LEU:HD12 | 63:Ao:538:MET:HG3  | 1.96                     | 0.48              |
| 72:B8:110:VAL:O    | 72:B8:114:PHE:HB2  | 2.13                     | 0.48              |
| 31:BA:1518:A:H2'   | 31:BA:1519:U:C6    | 2.49                     | 0.48              |
| 75:BC:177:ASP:OD1  | 75:BC:177:ASP:N    | 2.45                     | 0.48              |
| 81:BK:33:PRO:HA    | 81:BK:35:LEU:H     | 1.78                     | 0.48              |
| 84:BP:193:PHE:HE2  | 84:BP:200:ILE:HG12 | 1.79                     | 0.48              |
| 5:BW:159:ARG:HD2   | 31:BA:294:G:H5'    | 1.94                     | 0.48              |
| 7:BY:94:HIS:HE2    | 31:BA:140:A:P      | 2.37                     | 0.48              |
| 10:Bc:76:PHE:HB3   | 10:Bc:78:MET:HE2   | 1.95                     | 0.48              |
| 12:Be:32:LYS:NZ    | 31:BA:35:A:OP1     | 2.31                     | 0.48              |
| 31:AA:58:U:H3      | 59:Aj:57:ASP:CG    | 2.22                     | 0.48              |
| 31:AA:328:A:OP1    | 35:AF:90:ARG:NH2   | 2.35                     | 0.48              |
| 31:AA:348:A:H5''   | 38:AK:121:ASN:HD22 | 1.78                     | 0.48              |
| 33:AC:113:ARG:HH11 | 37:AJ:165:PRO:HA   | 1.79                     | 0.48              |
| 36:AG:215:ASN:HA   | 36:AG:220:ILE:HG13 | 1.96                     | 0.48              |
| 53:Ae:370:GLN:O    | 53:Ae:374:ARG:HG2  | 2.14                     | 0.48              |
| 59:Aj:68:LEU:HD12  | 59:Aj:71:LEU:HD12  | 1.96                     | 0.48              |
| 69:B5:163:GLU:OE1  | 69:B5:181:ARG:NH2  | 2.47                     | 0.48              |
| 31:BA:53:U:N3      | 31:BA:62:C:O2      | 2.36                     | 0.48              |
| 31:BA:908:A:H62    | 31:BA:912:U:H3     | 1.60                     | 0.48              |
| 75:BC:221:ARG:HD2  | 75:BC:235:TYR:HB3  | 1.95                     | 0.48              |
| 75:BC:481:LYS:HB2  | 75:BC:494:SER:HB2  | 1.95                     | 0.48              |
| 75:BC:488:ASN:HD22 | 75:BC:522:LYS:HE3  | 1.78                     | 0.48              |
| 80:BJ:33:VAL:HB    | 85:BQ:69:LEU:HD13  | 1.94                     | 0.48              |
| 5:BW:46:SER:N      | 31:BA:3:C:OP2      | 2.47                     | 0.48              |
| 8:Ba:84:HIS:HE1    | 8:Ba:86:LYS:HB3    | 1.79                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:Ba:361:THR:OG1   | 8:Ba:363:ASP:OD1   | 2.30                     | 0.48              |
| 13:Bf:71:HIS:HA    | 14:Bg:141:GLY:H    | 1.77                     | 0.48              |
| 30:Bx:82:ASN:CG    | 31:BA:574:A:H61    | 2.21                     | 0.48              |
| 31:AA:562:A:H8     | 31:AA:708:A:H61    | 1.60                     | 0.48              |
| 31:AA:641:A:H2'    | 31:AA:642:G:C8     | 2.48                     | 0.48              |
| 35:AF:42:LEU:HB2   | 35:AF:63:TYR:HB2   | 1.96                     | 0.48              |
| 41:AO:144:MET:HE1  | 41:AO:150:ASP:HB3  | 1.95                     | 0.48              |
| 53:Ae:119:ILE:HG23 | 53:Ae:124:ASP:HB2  | 1.95                     | 0.48              |
| 56:Ag:103:PRO:HG3  | 56:Ag:344:VAL:HG23 | 1.95                     | 0.48              |
| 60:Ak:213:ARG:NH1  | 60:Ak:223:TYR:OH   | 2.46                     | 0.48              |
| 75:BC:48:ASN:HB3   | 75:BC:138:LEU:HD22 | 1.95                     | 0.48              |
| 75:BC:523:VAL:HG13 | 75:BC:693:LEU:HD23 | 1.96                     | 0.48              |
| 78:BF:262:THR:HG22 | 78:BF:264:PRO:HD2  | 1.94                     | 0.48              |
| 87:BS:86:THR:O     | 87:BS:120:ARG:NH1  | 2.47                     | 0.48              |
| 14:Bg:93:SER:O     | 14:Bg:97:ILE:HG12  | 2.13                     | 0.48              |
| 25:Bt:16:GLN:OE1   | 25:Bt:23:ARG:NH1   | 2.44                     | 0.48              |
| 28:B0:144:LEU:HD22 | 87:BS:44:VAL:HG11  | 1.95                     | 0.48              |
| 31:AA:869:A:N7     | 31:AA:900:A:N6     | 2.61                     | 0.48              |
| 32:AB:151:ALA:HB3  | 45:AU:87:CYS:HB3   | 1.96                     | 0.48              |
| 45:AU:15:GLN:HG2   | 45:AU:16:GLU:HG2   | 1.96                     | 0.48              |
| 55:Af:81:PHE:HA    | 55:Af:84:MET:HG2   | 1.95                     | 0.48              |
| 63:Ao:646:GLU:OE1  | 63:Ao:647:GLY:N    | 2.45                     | 0.48              |
| 31:BA:316:U:H2'    | 31:BA:317:A:C8     | 2.49                     | 0.48              |
| 31:BA:972:C:C2     | 31:BA:973:A:C8     | 3.02                     | 0.48              |
| 76:BD:128:ILE:HD11 | 76:BD:144:ALA:HB2  | 1.95                     | 0.48              |
| 83:BO:52:HIS:CD2   | 83:BO:53:ARG:HG3   | 2.49                     | 0.48              |
| 84:BP:55:GLY:H     | 84:BP:59:ARG:NH1   | 2.12                     | 0.48              |
| 2:BT:165:GLU:OE2   | 77:BE:116:LYS:NZ   | 2.38                     | 0.48              |
| 15:Bh:166:VAL:HG11 | 15:Bh:192:ARG:HG3  | 1.96                     | 0.48              |
| 15:Bh:184:PHE:O    | 15:Bh:186:VAL:HG23 | 2.13                     | 0.48              |
| 25:Bt:97:VAL:HG23  | 25:Bt:98:THR:HG23  | 1.95                     | 0.48              |
| 26:Bu:64:ASP:HA    | 26:Bu:67:GLN:HE21  | 1.79                     | 0.48              |
| 31:AA:210:U:H2'    | 31:AA:211:A:C8     | 2.49                     | 0.48              |
| 31:AA:887:U:H2'    | 31:AA:888:A:H8     | 1.79                     | 0.48              |
| 34:AE:282:ILE:HG23 | 34:AE:353:LEU:HB3  | 1.95                     | 0.48              |
| 44:AR:93:TYR:HH    | 44:AR:141:TYR:HH   | 1.59                     | 0.48              |
| 61:Am:56:TRP:HB3   | 61:Am:61:PHE:CD1   | 2.49                     | 0.48              |
| 31:BA:1262:A:O2'   | 31:BA:1423:C:OP1   | 2.25                     | 0.48              |
| 78:BF:123:GLY:HA2  | 78:BF:141:ILE:HG12 | 1.95                     | 0.48              |
| 80:BJ:110:LEU:HB3  | 81:BK:132:LEU:HB3  | 1.96                     | 0.48              |
| 1:AI:206:LEU:HD12  | 1:AI:219:TYR:HD1   | 1.78                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 9:Bb:110:LEU:HD21  | 87:BS:113:LYS:HG2  | 1.95                     | 0.47              |
| 10:Bc:103:ALA:O    | 10:Bc:110:TRP:N    | 2.47                     | 0.47              |
| 25:Bt:14:GLY:N     | 31:BA:1279:G:H5''  | 2.29                     | 0.47              |
| 30:Bx:174:MET:HE1  | 82:BN:75:LYS:HB2   | 1.96                     | 0.47              |
| 31:AA:235:A:C6     | 64:Ap:82:LYS:HA    | 2.49                     | 0.47              |
| 31:AA:647:A:C5     | 45:AU:82:ASP:HB3   | 2.49                     | 0.47              |
| 34:AE:192:GLY:H    | 34:AE:201:VAL:HG12 | 1.79                     | 0.47              |
| 37:AJ:74:LYS:HB2   | 37:AJ:177:LEU:HD21 | 1.94                     | 0.47              |
| 46:AY:64:U:O4      | 46:AY:65:A:N6      | 2.45                     | 0.47              |
| 53:Ae:311:GLU:HA   | 53:Ae:388:VAL:HG21 | 1.96                     | 0.47              |
| 63:Ao:559:LYS:HD3  | 63:Ao:598:MET:HE2  | 1.95                     | 0.47              |
| 65:LL:185:LYS:HG3  | 65:LL:195:VAL:HB   | 1.95                     | 0.47              |
| 31:BA:219:A:H2'    | 31:BA:220:G:C8     | 2.48                     | 0.47              |
| 31:BA:434:U:H2'    | 31:BA:435:C:C6     | 2.48                     | 0.47              |
| 31:BA:512:A:C6     | 75:BC:675:ILE:HB   | 2.49                     | 0.47              |
| 31:BA:988:U:H5'    | 77:BE:229:ALA:HB3  | 1.96                     | 0.47              |
| 31:BA:1476:A:H2'   | 31:BA:1477:A:C8    | 2.49                     | 0.47              |
| 75:BC:207:LEU:O    | 75:BC:211:PHE:N    | 2.46                     | 0.47              |
| 80:BJ:41:HIS:CD2   | 80:BJ:43:GLU:H     | 2.32                     | 0.47              |
| 3:BU:112:THR:H     | 14:Bg:127:GLN:HE22 | 1.62                     | 0.47              |
| 8:Ba:236:LEU:HD23  | 8:Ba:341:VAL:HG22  | 1.96                     | 0.47              |
| 10:Bc:156:LYS:HE2  | 13:Bf:89:ASP:H     | 1.79                     | 0.47              |
| 17:Bj:133:LEU:HD22 | 68:B4:64:THR:HG21  | 1.95                     | 0.47              |
| 31:AA:815:U:H2'    | 31:AA:816:U:H6     | 1.80                     | 0.47              |
| 33:AC:85:ARG:HH21  | 60:Ak:162:GLY:HA3  | 1.79                     | 0.47              |
| 46:AY:15:A:O2'     | 46:AY:16:A:N3      | 2.45                     | 0.47              |
| 65:LL:159:VAL:HG21 | 75:BC:255:GLU:HB3  | 1.96                     | 0.47              |
| 31:BA:314:U:H2'    | 31:BA:315:G:H8     | 1.79                     | 0.47              |
| 31:BA:1326:A:O2'   | 31:BA:1328:G:OP2   | 2.28                     | 0.47              |
| 75:BC:679:ASP:O    | 81:BK:33:PRO:HD2   | 2.14                     | 0.47              |
| 82:BN:62:THR:HB    | 82:BN:129:PRO:HA   | 1.95                     | 0.47              |
| 4:BV:106:ALA:HB1   | 4:BV:122:ASN:HD21  | 1.79                     | 0.47              |
| 5:BW:123:GLN:NE2   | 5:BW:135:ARG:O     | 2.47                     | 0.47              |
| 7:BY:21:TYR:CZ     | 7:BY:82:GLN:HG2    | 2.49                     | 0.47              |
| 12:Be:126:PHE:CD2  | 12:Be:133:PHE:HB3  | 2.49                     | 0.47              |
| 20:Bm:76:LYS:HE2   | 20:Bm:83:VAL:HG21  | 1.97                     | 0.47              |
| 23:Bp:10:LEU:O     | 23:Bp:46:ASN:ND2   | 2.47                     | 0.47              |
| 31:AA:131:U:O2'    | 43:AQ:23:GLN:NE2   | 2.48                     | 0.47              |
| 31:AA:343:U:H2'    | 31:AA:344:G:O4'    | 2.14                     | 0.47              |
| 31:AA:454:A:HO2'   | 31:AA:936:C:HO2'   | 1.59                     | 0.47              |
| 31:AA:942:G:N2     | 31:AA:945:A:OP2    | 2.44                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 44:AR:137:CYS:O    | 52:Ad:193:ARG:NH2  | 2.39                     | 0.47              |
| 57:Ah:329:TYR:O    | 57:Ah:369:ARG:NH2  | 2.47                     | 0.47              |
| 60:Ak:63:ALA:HB3   | 60:Ak:66:GLN:HB2   | 1.96                     | 0.47              |
| 69:B5:144:GLN:HE22 | 69:B5:175:ILE:HA   | 1.79                     | 0.47              |
| 31:BA:877:U:O2'    | 31:BA:965:A:OP2    | 2.22                     | 0.47              |
| 8:Ba:280:GLN:HG2   | 29:Bw:152:ARG:NE   | 2.28                     | 0.47              |
| 17:Bj:59:VAL:HG21  | 17:Bj:136:ARG:HD2  | 1.96                     | 0.47              |
| 28:B0:76:HIS:O     | 28:B0:130:PHE:HA   | 2.14                     | 0.47              |
| 30:Bx:70:CYS:HB3   | 30:Bx:73:CYS:HB2   | 1.96                     | 0.47              |
| 31:AA:23:U:H2'     | 31:AA:24:C:H6      | 1.79                     | 0.47              |
| 31:AA:216:A:N7     | 31:AA:273:A:O2'    | 2.38                     | 0.47              |
| 31:AA:299:U:H2'    | 31:AA:300:G:C8     | 2.49                     | 0.47              |
| 41:AO:172:ARG:NH2  | 43:AQ:60:VAL:O     | 2.37                     | 0.47              |
| 52:Ad:64:ARG:HA    | 52:Ad:67:VAL:HG22  | 1.94                     | 0.47              |
| 56:Ag:335:ALA:HA   | 60:Ak:263:ASN:HD21 | 1.78                     | 0.47              |
| 31:BA:108:A:O4'    | 31:BA:110:A:N6     | 2.48                     | 0.47              |
| 31:BA:571:A:N3     | 82:BN:111:MET:HG2  | 2.29                     | 0.47              |
| 31:BA:745:A:H3'    | 31:BA:746:U:H5''   | 1.97                     | 0.47              |
| 31:BA:1060:C:H2'   | 31:BA:1061:U:H6    | 1.79                     | 0.47              |
| 74:BB:1:G:O6       | 74:BB:70:A:N6      | 2.47                     | 0.47              |
| 75:BC:126:ASP:HB3  | 75:BC:500:HIS:HB2  | 1.96                     | 0.47              |
| 75:BC:384:ILE:HD11 | 75:BC:423:ILE:HD11 | 1.95                     | 0.47              |
| 75:BC:393:VAL:HG11 | 75:BC:423:ILE:HD13 | 1.96                     | 0.47              |
| 77:BE:212:GLY:HA2  | 77:BE:262:GLY:HA3  | 1.97                     | 0.47              |
| 77:BE:276:ILE:HB   | 77:BE:332:LEU:HB2  | 1.96                     | 0.47              |
| 78:BF:212:TRP:O    | 78:BF:258:THR:OG1  | 2.32                     | 0.47              |
| 7:BY:170:TRP:O     | 12:Be:75:ARG:NH2   | 2.48                     | 0.47              |
| 22:Bo:91:TRP:CD2   | 25:Bt:58:GLN:HG2   | 2.49                     | 0.47              |
| 26:Bu:63:ASP:OD1   | 26:Bu:63:ASP:N     | 2.44                     | 0.47              |
| 26:Bu:102:PHE:CZ   | 26:Bu:132:LEU:HD23 | 2.49                     | 0.47              |
| 29:Bw:145:LEU:HD22 | 29:Bw:402:ASN:HA   | 1.97                     | 0.47              |
| 31:AA:875:A:H61    | 31:AA:893:A:N6     | 2.12                     | 0.47              |
| 31:AA:956:G:H2'    | 31:AA:957:A:H8     | 1.80                     | 0.47              |
| 34:AE:289:THR:HG22 | 34:AE:290:ILE:H    | 1.79                     | 0.47              |
| 34:AE:374:ARG:HB3  | 34:AE:377:CYS:HB2  | 1.95                     | 0.47              |
| 46:AV:69:C:H5''    | 31:BA:1425:A:OP1   | 2.13                     | 0.47              |
| 50:Ab:11:SER:HB2   | 50:Ab:44:PRO:HG2   | 1.97                     | 0.47              |
| 64:Ap:189:PRO:HB3  | 64:Ap:193:LEU:HD23 | 1.97                     | 0.47              |
| 65:CL:82:LEU:HD13  | 65:DL:67:LEU:HD13  | 1.96                     | 0.47              |
| 66:B2:128:MET:HE3  | 66:B2:131:PRO:HA   | 1.96                     | 0.47              |
| 31:BA:52:A:O2'     | 31:BA:245:A:N1     | 2.48                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:BA:1338:G:H2'   | 31:BA:1339:A:H8    | 1.80                     | 0.47              |
| 31:BA:1466:G:H2'   | 31:BA:1467:G:O4'   | 2.15                     | 0.47              |
| 31:BA:1531:C:H3'   | 31:BA:1532:U:H5''  | 1.97                     | 0.47              |
| 75:BC:426:ALA:HB2  | 75:BC:431:PHE:CZ   | 2.49                     | 0.47              |
| 78:BF:220:ASP:OD1  | 78:BF:221:LEU:N    | 2.45                     | 0.47              |
| 3:BU:137:GLU:HB2   | 3:BU:138:PRO:HD3   | 1.96                     | 0.47              |
| 4:BV:100:PHE:HD2   | 14:Bg:126:ILE:HD13 | 1.78                     | 0.47              |
| 5:BW:77:GLN:H      | 5:BW:171:HIS:CD2   | 2.31                     | 0.47              |
| 8:Ba:392:ILE:HG12  | 8:Ba:397:VAL:HG22  | 1.97                     | 0.47              |
| 10:Bc:101:ILE:HD12 | 10:Bc:126:THR:HA   | 1.97                     | 0.47              |
| 17:Bj:58:LEU:HD12  | 17:Bj:153:LEU:HD22 | 1.96                     | 0.47              |
| 31:AA:328:A:H2'    | 31:AA:329:A:C8     | 2.48                     | 0.47              |
| 53:Ae:218:THR:HG23 | 53:Ae:252:GLY:HA2  | 1.96                     | 0.47              |
| 53:Ae:242:ARG:NE   | 53:Ae:282:ALA:O    | 2.41                     | 0.47              |
| 56:Ag:103:PRO:HA   | 56:Ag:342:ILE:HD11 | 1.96                     | 0.47              |
| 31:BA:645:U:H2'    | 31:BA:646:A:H8     | 1.79                     | 0.47              |
| 31:BA:1420:A:H8    | 31:BA:1420:A:OP2   | 1.98                     | 0.47              |
| 31:BA:1502:U:H2'   | 31:BA:1503:C:C6    | 2.50                     | 0.47              |
| 75:BC:54:HIS:ND1   | 75:BC:154:GLN:HB3  | 2.29                     | 0.47              |
| 76:BD:203:ARG:HH21 | 76:BD:206:GLN:HE22 | 1.63                     | 0.47              |
| 4:BV:108:HIS:ND1   | 31:BA:480:G:OP2    | 2.48                     | 0.47              |
| 7:BY:18:ASN:HA     | 7:BY:43:ARG:HD3    | 1.96                     | 0.47              |
| 8:Ba:293:PHE:HE1   | 8:Ba:344:SER:HB2   | 1.80                     | 0.47              |
| 21:Bn:77:PRO:HA    | 31:BA:16:A:H5'     | 1.96                     | 0.47              |
| 30:Bx:58:GLN:OE1   | 82:BN:171:SER:OG   | 2.33                     | 0.47              |
| 31:AA:364:U:H2'    | 31:AA:365:A:H8     | 1.78                     | 0.47              |
| 31:AA:941:U:H2'    | 31:AA:942:G:H8     | 1.77                     | 0.47              |
| 32:AB:238:ASN:ND2  | 32:AB:241:SER:OG   | 2.48                     | 0.47              |
| 34:AE:136:ARG:N    | 58:Ai:67:PHE:O     | 2.47                     | 0.47              |
| 34:AE:176:ARG:HD3  | 58:Ai:84:ARG:HH12  | 1.79                     | 0.47              |
| 40:AN:56:SER:O     | 40:AN:60:ASN:ND2   | 2.47                     | 0.47              |
| 46:AV:56:C:H2'     | 46:AV:57:C:C6      | 2.49                     | 0.47              |
| 60:Ak:164:SER:HA   | 63:Ao:134:GLU:HG2  | 1.96                     | 0.47              |
| 63:Ao:469:CYS:SG   | 63:Ao:470:PHE:N    | 2.88                     | 0.47              |
| 67:B3:93:LYS:O     | 67:B3:96:THR:OG1   | 2.33                     | 0.47              |
| 31:BA:247:C:H2'    | 31:BA:248:A:C8     | 2.49                     | 0.47              |
| 31:BA:421:U:H2'    | 31:BA:422:U:C6     | 2.50                     | 0.47              |
| 31:BA:733:A:OP1    | 76:BD:102:GLN:NE2  | 2.48                     | 0.47              |
| 31:BA:742:U:H2'    | 31:BA:743:U:C6     | 2.49                     | 0.47              |
| 31:BA:1357:C:H3'   | 31:BA:1358:G:H5''  | 1.96                     | 0.47              |
| 75:BC:70:THR:HG22  | 75:BC:111:TRP:CE3  | 2.50                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 81:BK:20:ILE:HD11  | 81:BK:42:ARG:HG3   | 1.96                     | 0.47              |
| 1:AI:81:PHE:HZ     | 1:AI:101:GLN:HE22  | 1.63                     | 0.47              |
| 1:AI:158:TYR:CZ    | 1:AI:218:ASP:HB3   | 2.49                     | 0.47              |
| 1:AI:305:PHE:HB3   | 1:AI:310:ASP:HB2   | 1.97                     | 0.47              |
| 10:Bc:61:LYS:HG2   | 16:Bi:275:PRO:HB3  | 1.96                     | 0.47              |
| 11:Bd:129:ARG:HH22 | 17:Bj:56:PRO:HG3   | 1.80                     | 0.47              |
| 18:Bk:85:ASP:OD1   | 18:Bk:85:ASP:N     | 2.47                     | 0.47              |
| 25:Bt:15:ARG:HA    | 31:BA:1024:G:OP1   | 2.14                     | 0.47              |
| 25:Bt:24:PRO:HG2   | 30:Bx:169:TRP:HB2  | 1.97                     | 0.47              |
| 25:Bt:44:GLU:OE2   | 67:B3:120:LYS:NZ   | 2.36                     | 0.47              |
| 31:AA:438:C:H2'    | 31:AA:439:A:H8     | 1.78                     | 0.47              |
| 31:AA:616:C:H2'    | 31:AA:617:C:C6     | 2.50                     | 0.47              |
| 31:AA:750:G:H21    | 31:AA:777:A:H62    | 1.61                     | 0.47              |
| 35:AF:11:LYS:HB3   | 35:AF:13:MET:HE3   | 1.97                     | 0.47              |
| 35:AF:31:ASP:OD1   | 52:Ad:170:ARG:NH2  | 2.48                     | 0.47              |
| 63:Ao:258:ASN:HD22 | 63:Ao:285:LEU:HA   | 1.78                     | 0.47              |
| 72:B8:136:LYS:HB3  | 72:B8:140:ARG:HD3  | 1.97                     | 0.47              |
| 31:BA:120:C:H2'    | 31:BA:121:C:H6     | 1.79                     | 0.47              |
| 31:BA:499:C:H1'    | 31:BA:551:A:H2     | 1.78                     | 0.47              |
| 31:BA:551:A:H5'    | 80:BJ:150:HIS:ND1  | 2.30                     | 0.47              |
| 31:BA:731:U:O2'    | 31:BA:732:A:O5'    | 2.32                     | 0.47              |
| 31:BA:1079:U:H2'   | 31:BA:1080:A:C8    | 2.50                     | 0.47              |
| 31:BA:1195:A:N6    | 31:BA:1208:A:O2'   | 2.48                     | 0.47              |
| 31:BA:1452:C:H2'   | 31:BA:1453:U:C6    | 2.50                     | 0.47              |
| 78:BF:216:VAL:HG22 | 78:BF:258:THR:HB   | 1.96                     | 0.47              |
| 16:Bi:122:ILE:HG23 | 16:Bi:132:PHE:HE2  | 1.80                     | 0.47              |
| 31:AA:177:U:H2'    | 31:AA:178:G:H8     | 1.80                     | 0.47              |
| 31:AA:729:A:H2'    | 31:AA:730:C:O4'    | 2.15                     | 0.47              |
| 34:AE:225:VAL:HA   | 34:AE:243:VAL:HG12 | 1.95                     | 0.47              |
| 36:AG:173:PRO:HB3  | 61:Am:73:PHE:CZ    | 2.50                     | 0.47              |
| 70:B6:44:LEU:HB3   | 70:B6:53:LYS:HE3   | 1.96                     | 0.47              |
| 31:BA:193:U:H2'    | 31:BA:194:G:C8     | 2.50                     | 0.47              |
| 31:BA:1448:A:H2'   | 31:BA:1449:U:C6    | 2.49                     | 0.47              |
| 75:BC:68:TYR:HD1   | 75:BC:73:ILE:HG22  | 1.80                     | 0.47              |
| 77:BE:50:ASP:HB3   | 86:BR:139:ARG:HH12 | 1.79                     | 0.47              |
| 10:Bc:75:VAL:HB    | 16:Bi:282:ILE:HB   | 1.97                     | 0.47              |
| 11:Bd:85:HIS:CE1   | 68:B4:38:ARG:HH21  | 2.33                     | 0.47              |
| 15:Bh:98:ILE:HG12  | 15:Bh:119:LEU:HD12 | 1.97                     | 0.47              |
| 19:Bl:90:ARG:NH2   | 78:BF:279:ARG:H    | 2.13                     | 0.47              |
| 31:AA:567:C:H2'    | 31:AA:568:G:C8     | 2.43                     | 0.47              |
| 31:AA:961:C:H41    | 61:Am:101:PRO:HG3  | 1.80                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 41:AO:87:ASP:OD1   | 41:AO:87:ASP:N     | 2.45                     | 0.47              |
| 42:AP:108:GLU:HG2  | 64:Ap:231:PRO:HG3  | 1.97                     | 0.47              |
| 62:An:130:ILE:HD13 | 62:An:133:ILE:HD12 | 1.97                     | 0.47              |
| 63:Ao:379:ILE:HD12 | 63:Ao:396:ILE:HG23 | 1.96                     | 0.47              |
| 66:B2:172:ARG:HE   | 66:B2:203:ALA:HB2  | 1.80                     | 0.47              |
| 31:BA:404:C:N4     | 31:BA:405:C:H42    | 2.13                     | 0.47              |
| 75:BC:319:ASN:OD1  | 75:BC:321:SER:OG   | 2.26                     | 0.47              |
| 78:BF:84:PRO:HA    | 78:BF:88:SER:HB3   | 1.97                     | 0.47              |
| 80:BJ:65:LEU:HD12  | 80:BJ:66:PRO:HD2   | 1.97                     | 0.47              |
| 1:AI:235:GLY:H     | 1:AI:238:GLU:HB2   | 1.80                     | 0.46              |
| 3:BU:34:ARG:HH21   | 31:BA:1014:A:H5''  | 1.78                     | 0.46              |
| 11:Bd:103:LEU:HD12 | 11:Bd:114:HIS:CE1  | 2.50                     | 0.46              |
| 12:Be:28:ARG:HD2   | 31:BA:670:A:H5''   | 1.96                     | 0.46              |
| 13:Bf:46:LYS:O     | 13:Bf:63:PRO:HD2   | 2.15                     | 0.46              |
| 17:Bj:215:PHE:HB3  | 17:Bj:268:TYR:CE1  | 2.50                     | 0.46              |
| 20:Bm:66:ASP:OD1   | 20:Bm:69:SER:HB2   | 2.14                     | 0.46              |
| 24:Bq:65:PRO:HB3   | 81:BK:165:ALA:HB2  | 1.98                     | 0.46              |
| 29:Bw:242:PRO:HB3  | 29:Bw:424:LYS:HG2  | 1.97                     | 0.46              |
| 31:AA:604:U:O4'    | 58:Ai:95:ARG:NH1   | 2.48                     | 0.46              |
| 33:AC:116:GLN:HB3  | 33:AC:150:PRO:HG2  | 1.97                     | 0.46              |
| 34:AE:317:HIS:CD2  | 34:AE:319:ALA:H    | 2.34                     | 0.46              |
| 36:AG:242:TRP:HD1  | 61:Am:84:ARG:HH22  | 1.62                     | 0.46              |
| 51:Ac:105:ILE:HG13 | 51:Ac:106:LEU:HG   | 1.97                     | 0.46              |
| 65:LL:143:VAL:HG22 | 75:BC:269:LEU:HD22 | 1.97                     | 0.46              |
| 31:BA:147:U:H2'    | 31:BA:148:A:O4'    | 2.15                     | 0.46              |
| 31:BA:266:C:N4     | 31:BA:309:A:N1     | 2.63                     | 0.46              |
| 31:BA:1060:C:H2'   | 31:BA:1061:U:C6    | 2.50                     | 0.46              |
| 74:BB:42:C:OP2     | 87:BS:85:ARG:NH2   | 2.44                     | 0.46              |
| 11:Bd:41:ILE:HG22  | 11:Bd:43:ASP:H     | 1.79                     | 0.46              |
| 19:Bl:142:GLU:OE2  | 84:BP:11:ARG:NH2   | 2.47                     | 0.46              |
| 31:AA:13:U:H2'     | 31:AA:14:C:C6      | 2.50                     | 0.46              |
| 31:AA:531:U:O2'    | 31:AA:929:A:N7     | 2.47                     | 0.46              |
| 41:AO:140:TYR:HB2  | 41:AO:157:LEU:HD13 | 1.97                     | 0.46              |
| 42:AP:59:ASN:ND2   | 42:AP:63:GLU:O     | 2.48                     | 0.46              |
| 67:B3:40:ARG:NH1   | 31:BA:410:U:OP2    | 2.47                     | 0.46              |
| 73:B9:74:ARG:NH1   | 31:BA:545:U:O3'    | 2.48                     | 0.46              |
| 31:BA:727:A:O2'    | 31:BA:728:C:O4'    | 2.32                     | 0.46              |
| 84:BP:223:LEU:HD21 | 84:BP:262:PRO:HB3  | 1.97                     | 0.46              |
| 86:BR:125:GLU:OE2  | 86:BR:129:ASN:ND2  | 2.45                     | 0.46              |
| 1:AI:350:ALA:HB1   | 1:AI:370:LEU:HB3   | 1.98                     | 0.46              |
| 7:BY:110:PRO:HD3   | 16:Bi:166:GLU:HG2  | 1.95                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:Ba:125:LYS:NZ    | 8:Ba:366:SER:O     | 2.47                     | 0.46              |
| 17:Bj:159:LEU:HD11 | 17:Bj:252:HIS:HB2  | 1.97                     | 0.46              |
| 31:AA:386:U:H2'    | 31:AA:387:C:C6     | 2.50                     | 0.46              |
| 31:AA:477:A:H2'    | 31:AA:478:A:C8     | 2.51                     | 0.46              |
| 32:AB:161:CYS:SG   | 32:AB:253:GLN:HA   | 2.55                     | 0.46              |
| 46:AY:9:C:O2'      | 46:AY:10:A:N7      | 2.43                     | 0.46              |
| 54:B1:91:TYR:OH    | 31:BA:61:U:OP1     | 2.24                     | 0.46              |
| 65:EL:75:THR:HG22  | 65:EL:78:GLU:HG2   | 1.98                     | 0.46              |
| 31:BA:450:U:C2     | 31:BA:451:U:C5     | 3.04                     | 0.46              |
| 31:BA:484:A:OP2    | 31:BA:583:A:N6     | 2.40                     | 0.46              |
| 31:BA:1544:A:H5'   | 77:BE:303:LYS:HG3  | 1.96                     | 0.46              |
| 75:BC:433:ASP:OD1  | 75:BC:433:ASP:N    | 2.47                     | 0.46              |
| 75:BC:488:ASN:HB3  | 75:BC:522:LYS:HE3  | 1.98                     | 0.46              |
| 78:BF:56:PRO:HG2   | 78:BF:59:ARG:HB3   | 1.97                     | 0.46              |
| 79:BI:139:LEU:O    | 79:BI:142:GLU:HG3  | 2.15                     | 0.46              |
| 84:BP:100:ARG:O    | 84:BP:104:LEU:HG   | 2.15                     | 0.46              |
| 85:BQ:75:PRO:HB3   | 85:BQ:241:TYR:CZ   | 2.50                     | 0.46              |
| 2:BT:225:LYS:O     | 2:BT:229:TRP:NE1   | 2.37                     | 0.46              |
| 9:Bb:59:ARG:NH2    | 87:BS:85:ARG:O     | 2.42                     | 0.46              |
| 21:Bn:126:LYS:HD2  | 84:BP:51:ARG:HD3   | 1.97                     | 0.46              |
| 28:B0:107:ASN:ND2  | 28:B0:109:SER:OG   | 2.48                     | 0.46              |
| 31:AA:942:G:H2'    | 31:AA:944:A:OP2    | 2.16                     | 0.46              |
| 35:AF:115:GLU:HG3  | 35:AF:116:LYS:H    | 1.80                     | 0.46              |
| 42:AP:114:ARG:HH21 | 64:Ap:237:GLU:HA   | 1.80                     | 0.46              |
| 54:B1:91:TYR:CZ    | 79:BI:79:VAL:HG11  | 2.51                     | 0.46              |
| 61:Am:64:GLU:OE1   | 61:Am:64:GLU:N     | 2.49                     | 0.46              |
| 67:B3:109:LYS:O    | 67:B3:113:VAL:HG22 | 2.16                     | 0.46              |
| 31:BA:301:U:H2'    | 31:BA:302:A:C8     | 2.49                     | 0.46              |
| 75:BC:500:HIS:O    | 75:BC:503:ILE:HG13 | 2.16                     | 0.46              |
| 80:BJ:44:ARG:NH1   | 85:BQ:234:ASP:OD2  | 2.44                     | 0.46              |
| 87:BS:154:ALA:HA   | 87:BS:159:LYS:HE3  | 1.98                     | 0.46              |
| 4:BV:76:GLU:OE1    | 4:BV:80:HIS:NE2    | 2.48                     | 0.46              |
| 6:BX:138:ASP:HB3   | 6:BX:141:ARG:HG2   | 1.96                     | 0.46              |
| 8:Ba:229:ARG:NE    | 8:Ba:231:ASN:HD21  | 2.14                     | 0.46              |
| 8:Ba:394:LYS:HA    | 31:BA:270:U:OP1    | 2.15                     | 0.46              |
| 10:Bc:61:LYS:HD2   | 10:Bc:77:VAL:HG12  | 1.98                     | 0.46              |
| 10:Bc:289:LEU:HD23 | 10:Bc:289:LEU:H    | 1.81                     | 0.46              |
| 11:Bd:57:ARG:NH2   | 17:Bj:79:ILE:O     | 2.48                     | 0.46              |
| 12:Be:126:PHE:HD2  | 12:Be:133:PHE:HB3  | 1.80                     | 0.46              |
| 15:Bh:156:LEU:HD21 | 15:Bh:228:LEU:HD12 | 1.97                     | 0.46              |
| 21:Bn:51:ARG:NE    | 31:BA:612:A:OP1    | 2.36                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 33:AC:76:LEU:HD13  | 37:AJ:81:LYS:HG3   | 1.97                     | 0.46              |
| 33:AC:123:VAL:O    | 33:AC:157:THR:HA   | 2.16                     | 0.46              |
| 57:Ah:350:LEU:HD13 | 57:Ah:361:LYS:HB3  | 1.98                     | 0.46              |
| 60:Ak:55:LEU:HD12  | 60:Ak:56:PRO:HD2   | 1.98                     | 0.46              |
| 60:Ak:249:ASP:OD1  | 60:Ak:249:ASP:N    | 2.44                     | 0.46              |
| 67:B3:74:SER:N     | 31:BA:472:U:OP2    | 2.49                     | 0.46              |
| 69:B5:181:ARG:NH1  | 69:B5:187:GLN:HA   | 2.30                     | 0.46              |
| 31:BA:204:G:H1'    | 31:BA:238:C:H5'    | 1.98                     | 0.46              |
| 31:BA:521:C:H2'    | 31:BA:522:A:C8     | 2.51                     | 0.46              |
| 31:BA:1569:A:H2'   | 31:BA:1570:C:C2    | 2.51                     | 0.46              |
| 81:BK:47:ASN:N     | 81:BK:47:ASN:OD1   | 2.48                     | 0.46              |
| 1:AI:78:ILE:HA     | 1:AI:128:PRO:HG2   | 1.97                     | 0.46              |
| 2:BT:86:ARG:HH12   | 31:BA:1557:C:H4'   | 1.81                     | 0.46              |
| 3:BU:73:THR:HG22   | 3:BU:83:TYR:HB2    | 1.97                     | 0.46              |
| 12:Be:51:ILE:HG22  | 12:Be:53:GLU:H     | 1.79                     | 0.46              |
| 19:Bl:54:PRO:HA    | 78:BF:291:CYS:HB3  | 1.96                     | 0.46              |
| 23:Bp:10:LEU:HD23  | 23:Bp:42:VAL:HG13  | 1.97                     | 0.46              |
| 31:AA:916:A:H2'    | 31:AA:917:C:O4'    | 2.16                     | 0.46              |
| 32:AB:78:PHE:HZ    | 32:AB:125:GLN:HG2  | 1.81                     | 0.46              |
| 54:B1:115:TYR:OH   | 54:B1:120:ASP:OD1  | 2.25                     | 0.46              |
| 60:Ak:58:ARG:O     | 60:Ak:62:MET:HG2   | 2.16                     | 0.46              |
| 65:EL:68:VAL:HG21  | 65:FL:85:LEU:HD23  | 1.96                     | 0.46              |
| 10:Bc:41:GLN:HB3   | 10:Bc:258:ILE:HD12 | 1.97                     | 0.46              |
| 23:Bp:13:VAL:HA    | 23:Bp:68:PHE:HB3   | 1.97                     | 0.46              |
| 29:Bw:278:ILE:HD11 | 29:Bw:333:GLN:HG2  | 1.96                     | 0.46              |
| 31:AA:616:C:H2'    | 31:AA:617:C:H6     | 1.80                     | 0.46              |
| 31:AA:618:G:N2     | 37:AJ:124:VAL:HG21 | 2.31                     | 0.46              |
| 31:AA:750:G:N2     | 31:AA:776:A:N7     | 2.64                     | 0.46              |
| 46:AV:44:U:H4'     | 46:AV:45:G:H5''    | 1.97                     | 0.46              |
| 31:BA:695:U:H3     | 31:BA:696:A:N6     | 2.14                     | 0.46              |
| 31:BA:864:U:H2'    | 31:BA:865:A:C8     | 2.51                     | 0.46              |
| 31:BA:1137:A:H2'   | 31:BA:1138:G:H8    | 1.80                     | 0.46              |
| 75:BC:465:LYS:HA   | 75:BC:468:LYS:HG2  | 1.96                     | 0.46              |
| 85:BQ:41:ASP:OD1   | 85:BQ:41:ASP:N     | 2.43                     | 0.46              |
| 11:Bd:38:LEU:HD23  | 11:Bd:38:LEU:H     | 1.80                     | 0.46              |
| 17:Bj:87:HIS:CE1   | 17:Bj:117:ALA:HB1  | 2.51                     | 0.46              |
| 31:AA:884:C:H5     | 53:Ae:143:TYR:HA   | 1.80                     | 0.46              |
| 35:AF:26:LEU:HD22  | 35:AF:36:VAL:HG21  | 1.98                     | 0.46              |
| 53:Ae:97:MET:HE1   | 53:Ae:131:TYR:HB3  | 1.98                     | 0.46              |
| 56:Ag:70:SER:OG    | 56:Ag:72:GLN:OE1   | 2.33                     | 0.46              |
| 56:Ag:364:TRP:NE1  | 56:Ag:394:CYS:O    | 2.48                     | 0.46              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 60:Ak:79:LYS:HD2  | 63:Ao:91:ASP:HB3   | 1.97                     | 0.46              |
| 65:GL:84:GLU:HA   | 65:GL:87:LYS:HG2   | 1.98                     | 0.46              |
| 31:BA:248:A:H2'   | 31:BA:249:G:C8     | 2.50                     | 0.46              |
| 78:BF:249:ASN:OD1 | 78:BF:249:ASN:N    | 2.49                     | 0.46              |
| 81:BK:30:ARG:H    | 81:BK:30:ARG:HD2   | 1.79                     | 0.46              |
| 82:BN:67:PHE:HB2  | 82:BN:72:TRP:NE1   | 2.30                     | 0.46              |
| 4:BV:168:THR:OG1  | 4:BV:169:GLU:N     | 2.49                     | 0.46              |
| 5:BW:78:ILE:HG22  | 5:BW:80:TYR:H      | 1.81                     | 0.46              |
| 8:Ba:153:ARG:HH22 | 29:Bw:191:ALA:HA   | 1.81                     | 0.46              |
| 15:Bh:72:ILE:HD13 | 15:Bh:178:LEU:HD23 | 1.98                     | 0.46              |
| 19:Bl:91:MET:HE3  | 31:BA:219:A:H5''   | 1.98                     | 0.46              |
| 31:AA:393:A:H5'   | 41:AO:133:LEU:HD21 | 1.97                     | 0.46              |
| 31:AA:551:G:H5'   | 31:AA:782:G:O6     | 2.16                     | 0.46              |
| 31:AA:761:U:O2'   | 31:AA:804:A:N3     | 2.40                     | 0.46              |
| 35:AF:105:CYS:HB2 | 44:AR:70:GLU:H     | 1.80                     | 0.46              |
| 53:Ae:180:ASP:OD1 | 53:Ae:180:ASP:N    | 2.49                     | 0.46              |
| 31:BA:175:C:H2'   | 31:BA:176:U:C6     | 2.51                     | 0.46              |
| 31:BA:498:A:H5''  | 31:BA:499:C:H5     | 1.81                     | 0.46              |
| 31:BA:794:A:H2'   | 31:BA:795:G:H8     | 1.81                     | 0.46              |
| 31:BA:1154:U:C2   | 31:BA:1155:G:C8    | 3.04                     | 0.46              |
| 80:BJ:225:GLN:HB3 | 80:BJ:226:PRO:HD3  | 1.97                     | 0.46              |
| 2:BT:112:TYR:CD1  | 2:BT:181:LYS:HE2   | 2.51                     | 0.46              |
| 9:Bb:62:GLU:OE1   | 87:BS:82:ARG:NH1   | 2.39                     | 0.46              |
| 10:Bc:179:ASP:HB3 | 10:Bc:290:VAL:HG11 | 1.98                     | 0.46              |
| 14:Bg:4:ARG:NH2   | 31:BA:167:G:O6     | 2.49                     | 0.46              |
| 17:Bj:152:LYS:HD2 | 17:Bj:157:LEU:HD21 | 1.97                     | 0.46              |
| 31:AA:22:U:H4'    | 64:Ap:83:GLY:HA3   | 1.98                     | 0.46              |
| 31:AA:277:A:H2'   | 31:AA:278:A:C8     | 2.51                     | 0.46              |
| 46:AY:11:G:H2'    | 46:AY:12:C:H6      | 1.81                     | 0.46              |
| 53:Ae:136:ARG:NH1 | 53:Ae:173:VAL:O    | 2.49                     | 0.46              |
| 63:Ao:434:LEU:O   | 63:Ao:438:VAL:HG23 | 2.16                     | 0.46              |
| 65:HL:85:LEU:HD12 | 65:HL:88:LYS:HD3   | 1.97                     | 0.46              |
| 31:BA:52:A:H4'    | 31:BA:245:A:H2     | 1.81                     | 0.46              |
| 31:BA:388:A:H2'   | 31:BA:389:A:C8     | 2.49                     | 0.46              |
| 31:BA:644:G:O2'   | 31:BA:1007:G:O6    | 2.33                     | 0.46              |
| 31:BA:1236:C:H2'  | 31:BA:1237:A:H8    | 1.80                     | 0.46              |
| 31:BA:1290:C:H4'  | 85:BQ:178:LEU:HD22 | 1.98                     | 0.46              |
| 78:BF:49:ARG:HG3  | 78:BF:263:LEU:HD22 | 1.98                     | 0.46              |
| 8:Ba:276:ASP:OD1  | 29:Bw:152:ARG:NH1  | 2.40                     | 0.45              |
| 8:Ba:360:ASN:HD22 | 8:Ba:372:ASN:HA    | 1.81                     | 0.45              |
| 11:Bd:89:ARG:HH22 | 74:BB:29:G:P       | 2.35                     | 0.45              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 18:Bk:195:LYS:HA  | 18:Bk:198:PHE:CD1  | 2.51                     | 0.45              |
| 30:Bx:82:ASN:OD1  | 31:BA:574:A:N6     | 2.39                     | 0.45              |
| 31:AA:57:A:C8     | 59:Aj:51:PRO:HB3   | 2.51                     | 0.45              |
| 34:AE:224:GLU:HB2 | 34:AE:342:MET:HG2  | 1.98                     | 0.45              |
| 46:AV:38:C:H2'    | 46:AV:39:G:H8      | 1.81                     | 0.45              |
| 56:Ag:240:GLY:HA3 | 56:Ag:291:ASN:HD22 | 1.81                     | 0.45              |
| 57:Ah:303:TRP:CZ2 | 60:Ak:165:ILE:HG12 | 2.51                     | 0.45              |
| 61:Am:72:ASP:OD1  | 61:Am:73:PHE:N     | 2.49                     | 0.45              |
| 31:BA:220:G:H1'   | 31:BA:231:C:H1'    | 1.98                     | 0.45              |
| 31:BA:871:A:OP2   | 31:BA:871:A:H8     | 1.98                     | 0.45              |
| 31:BA:1072:A:H2'  | 31:BA:1073:A:H8    | 1.81                     | 0.45              |
| 31:BA:1458:G:O2'  | 31:BA:1467:G:O6    | 2.29                     | 0.45              |
| 78:BF:68:SER:O    | 78:BF:210:ARG:NH2  | 2.47                     | 0.45              |
| 78:BF:220:ASP:HB2 | 78:BF:242:LEU:HD11 | 1.97                     | 0.45              |
| 8:Ba:207:ASN:HD21 | 8:Ba:229:ARG:HB3   | 1.80                     | 0.45              |
| 17:Bj:52:CYS:HB3  | 17:Bj:158:ILE:HD11 | 1.97                     | 0.45              |
| 31:AA:238:C:H2'   | 31:AA:239:U:C6     | 2.51                     | 0.45              |
| 31:AA:332:U:H2'   | 31:AA:333:A:H8     | 1.81                     | 0.45              |
| 36:AG:153:GLU:HA  | 36:AG:183:ALA:HB2  | 1.96                     | 0.45              |
| 56:Ag:207:TYR:CZ  | 56:Ag:241:ILE:HG23 | 2.51                     | 0.45              |
| 63:Ao:89:PHE:HE1  | 63:Ao:106:PHE:HB2  | 1.82                     | 0.45              |
| 63:Ao:257:LYS:HB3 | 63:Ao:260:HIS:HD2  | 1.81                     | 0.45              |
| 31:BA:993:U:H2'   | 31:BA:994:A:H8     | 1.82                     | 0.45              |
| 75:BC:76:MET:O    | 75:BC:77:HIS:ND1   | 2.49                     | 0.45              |
| 81:BK:102:ARG:NH1 | 81:BK:182:ASP:OD2  | 2.42                     | 0.45              |
| 2:BT:189:TYR:CD1  | 2:BT:243:ILE:HD11  | 2.52                     | 0.45              |
| 3:BU:114:LYS:HD3  | 13:Bf:45:CYS:SG    | 2.57                     | 0.45              |
| 4:BV:139:LEU:HD13 | 4:BV:148:LEU:HD23  | 1.97                     | 0.45              |
| 8:Ba:260:SER:OG   | 76:BD:146:GLY:O    | 2.35                     | 0.45              |
| 15:Bh:261:SER:OG  | 82:BN:16:ARG:O     | 2.29                     | 0.45              |
| 19:Bl:112:LYS:NZ  | 31:BA:217:A:OP1    | 2.49                     | 0.45              |
| 26:Bu:71:ILE:HG21 | 26:Bu:150:LEU:HD22 | 1.98                     | 0.45              |
| 37:AJ:80:VAL:HG21 | 37:AJ:91:TYR:CE2   | 2.51                     | 0.45              |
| 42:AP:21:LEU:HD22 | 42:AP:34:ILE:HG12  | 1.99                     | 0.45              |
| 49:Aa:190:ARG:NH2 | 49:Aa:258:GLU:OE1  | 2.49                     | 0.45              |
| 53:Ae:113:SER:HA  | 53:Ae:116:VAL:HG22 | 1.98                     | 0.45              |
| 54:B1:115:TYR:HB2 | 54:B1:122:ARG:HG2  | 1.98                     | 0.45              |
| 31:BA:150:A:N3    | 31:BA:198:U:O2'    | 2.45                     | 0.45              |
| 31:BA:230:G:H2'   | 31:BA:231:C:C6     | 2.52                     | 0.45              |
| 31:BA:611:U:H2'   | 31:BA:612:A:C8     | 2.52                     | 0.45              |
| 75:BC:402:HIS:C   | 75:BC:404:ASP:H    | 2.24                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 80:BJ:235:GLN:HE21 | 80:BJ:239:GLN:HE21 | 1.65                     | 0.45              |
| 82:BN:63:ARG:HA    | 82:BN:96:HIS:HE1   | 1.81                     | 0.45              |
| 1:AI:202:ILE:HG13  | 1:AI:205:GLU:H     | 1.79                     | 0.45              |
| 12:Be:82:THR:OG1   | 66:B2:90:GLN:NE2   | 2.43                     | 0.45              |
| 31:AA:387:C:C2     | 31:AA:388:U:C5     | 3.04                     | 0.45              |
| 31:AA:634:C:O2'    | 31:AA:650:A:N1     | 2.40                     | 0.45              |
| 44:AR:77:ASN:OD1   | 44:AR:77:ASN:N     | 2.48                     | 0.45              |
| 49:Aa:221:ARG:NH1  | 49:Aa:224:ARG:HE   | 2.14                     | 0.45              |
| 54:B1:42:HIS:CE1   | 54:B1:83:GLU:HB2   | 2.51                     | 0.45              |
| 56:Ag:54:ASP:N     | 56:Ag:54:ASP:OD1   | 2.50                     | 0.45              |
| 56:Ag:122:ARG:NH1  | 56:Ag:336:LEU:O    | 2.50                     | 0.45              |
| 56:Ag:154:ILE:HB   | 56:Ag:261:VAL:HA   | 1.98                     | 0.45              |
| 60:Ak:268:LEU:HD21 | 60:Ak:321:LEU:HD11 | 1.98                     | 0.45              |
| 61:Am:116:HIS:HD2  | 61:Am:117:VAL:HG23 | 1.81                     | 0.45              |
| 63:Ao:472:GLU:HG3  | 63:Ao:473:GLN:H    | 1.81                     | 0.45              |
| 31:BA:50:A:H2'     | 31:BA:51:A:C8      | 2.51                     | 0.45              |
| 31:BA:1022:G:H2'   | 31:BA:1023:U:C6    | 2.51                     | 0.45              |
| 31:BA:1050:C:N4    | 31:BA:1323:U:H1'   | 2.30                     | 0.45              |
| 74:BB:35:G:H2'     | 74:BB:36:A:C8      | 2.50                     | 0.45              |
| 77:BE:61:VAL:O     | 77:BE:65:VAL:HG23  | 2.17                     | 0.45              |
| 2:BT:96:ARG:HA     | 2:BT:99:MET:SD     | 2.56                     | 0.45              |
| 11:Bd:120:ARG:HD2  | 18:Bk:88:TYR:CE2   | 2.52                     | 0.45              |
| 31:AA:883:C:H1'    | 31:AA:886:A:C6     | 2.51                     | 0.45              |
| 33:AC:144:SER:HB3  | 33:AC:151:VAL:HG22 | 1.97                     | 0.45              |
| 60:Ak:66:GLN:NE2   | 63:Ao:81:ASP:OD1   | 2.50                     | 0.45              |
| 60:Ak:68:TRP:N     | 60:Ak:69:PRO:HD2   | 2.32                     | 0.45              |
| 60:Ak:184:LEU:HD12 | 60:Ak:188:ALA:HB1  | 1.99                     | 0.45              |
| 63:Ao:382:PHE:O    | 63:Ao:386:GLU:HB2  | 2.17                     | 0.45              |
| 72:B8:109:ALA:O    | 72:B8:113:ARG:HG2  | 2.16                     | 0.45              |
| 31:BA:203:A:O2'    | 31:BA:239:C:O2     | 2.29                     | 0.45              |
| 31:BA:343:C:H2'    | 31:BA:344:U:H6     | 1.81                     | 0.45              |
| 31:BA:491:U:H3'    | 31:BA:492:A:H5''   | 1.99                     | 0.45              |
| 31:BA:633:U:H5''   | 31:BA:634:G:H5''   | 1.99                     | 0.45              |
| 31:BA:1050:C:H2'   | 31:BA:1327:U:H4'   | 1.97                     | 0.45              |
| 75:BC:489:LYS:H    | 75:BC:489:LYS:HD2  | 1.81                     | 0.45              |
| 75:BC:681:VAL:HG13 | 75:BC:682:GLU:H    | 1.82                     | 0.45              |
| 8:Ba:409:GLU:HG3   | 8:Ba:413:LYS:HE3   | 1.99                     | 0.45              |
| 12:Be:25:ARG:O     | 71:B7:60:ASN:ND2   | 2.49                     | 0.45              |
| 16:Bi:189:LEU:HD12 | 16:Bi:217:HIS:HE2  | 1.82                     | 0.45              |
| 21:Bn:69:HIS:CD2   | 21:Bn:71:LYS:HG3   | 2.41                     | 0.45              |
| 31:AA:404:C:OP1    | 41:AO:151:LYS:NZ   | 2.50                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:AA:533:C:H2'    | 31:AA:534:U:C6     | 2.51                     | 0.45              |
| 31:AA:836:G:O2'    | 31:AA:928:A:OP1    | 2.34                     | 0.45              |
| 34:AE:292:HIS:HE1  | 34:AE:357:GLU:H    | 1.64                     | 0.45              |
| 35:AF:24:ARG:NH2   | 35:AF:87:ASP:OD2   | 2.50                     | 0.45              |
| 49:Aa:104:MET:HG2  | 49:Aa:290:PHE:HE1  | 1.82                     | 0.45              |
| 56:Ag:128:GLU:O    | 56:Ag:133:LYS:NZ   | 2.49                     | 0.45              |
| 59:Aj:98:THR:HG23  | 59:Aj:99:ARG:HG2   | 1.97                     | 0.45              |
| 59:Aj:132:GLU:OE1  | 59:Aj:205:ALA:N    | 2.43                     | 0.45              |
| 63:Ao:257:LYS:HG2  | 63:Ao:259:ALA:H    | 1.82                     | 0.45              |
| 66:B2:100:LEU:HB3  | 66:B2:144:LEU:HD11 | 1.99                     | 0.45              |
| 66:B2:226:ARG:NH2  | 31:BA:17:C:N3      | 2.54                     | 0.45              |
| 31:AA:50:U:H2'     | 31:AA:51:G:C8      | 2.47                     | 0.45              |
| 31:AA:122:C:H2'    | 31:AA:123:U:C6     | 2.51                     | 0.45              |
| 31:AA:763:A:H5''   | 40:AN:58:ARG:NH2   | 2.32                     | 0.45              |
| 31:AA:879:A:H5''   | 53:Ae:448:ARG:HH12 | 1.82                     | 0.45              |
| 31:AA:892:A:C5     | 59:Aj:21:LEU:HD21  | 2.52                     | 0.45              |
| 53:Ae:270:LEU:HD12 | 53:Ae:273:LYS:HD3  | 1.99                     | 0.45              |
| 70:B6:54:VAL:HB    | 70:B6:56:PHE:CE1   | 2.52                     | 0.45              |
| 31:BA:435:C:H2'    | 31:BA:436:U:C6     | 2.52                     | 0.45              |
| 31:BA:863:U:O2     | 76:BD:254:ASN:N    | 2.49                     | 0.45              |
| 31:BA:882:A:C5     | 31:BA:883:G:C8     | 3.05                     | 0.45              |
| 31:BA:1384:A:H2'   | 31:BA:1385:U:O4'   | 2.17                     | 0.45              |
| 31:BA:1385:U:O4    | 31:BA:1389:A:N7    | 2.49                     | 0.45              |
| 75:BC:328:ILE:HG13 | 75:BC:439:LEU:HA   | 1.99                     | 0.45              |
| 8:Ba:107:PHE:HB2   | 8:Ba:265:LEU:HD22  | 1.98                     | 0.45              |
| 16:Bi:125:ILE:HG12 | 16:Bi:252:LEU:HD11 | 1.99                     | 0.45              |
| 17:Bj:248:LYS:HG3  | 17:Bj:250:GLY:H    | 1.82                     | 0.45              |
| 31:AA:855:C:H2'    | 31:AA:856:U:C6     | 2.51                     | 0.45              |
| 40:AN:34:MET:HE3   | 58:Ai:52:TYR:CD2   | 2.51                     | 0.45              |
| 41:AO:171:LEU:HG   | 41:AO:179:PHE:HB2  | 1.98                     | 0.45              |
| 68:B4:43:ARG:NH1   | 68:B4:44:LEU:O     | 2.50                     | 0.45              |
| 69:B5:126:CYS:HA   | 69:B5:129:LYS:HE2  | 1.99                     | 0.45              |
| 31:BA:176:U:H2'    | 31:BA:177:U:C6     | 2.52                     | 0.45              |
| 31:BA:570:A:H2'    | 31:BA:571:A:H8     | 1.79                     | 0.45              |
| 31:BA:1330:U:H2'   | 31:BA:1331:G:O4'   | 2.17                     | 0.45              |
| 31:BA:1370:U:H2'   | 31:BA:1371:C:C6    | 2.52                     | 0.45              |
| 31:BA:1477:A:H2'   | 31:BA:1478:U:C6    | 2.51                     | 0.45              |
| 77:BE:55:GLU:HG3   | 86:BR:139:ARG:HG3  | 1.99                     | 0.45              |
| 84:BP:203:ARG:HH21 | 84:BP:262:PRO:HA   | 1.81                     | 0.45              |
| 1:AI:224:ARG:O     | 1:AI:227:GLU:HG3   | 2.15                     | 0.45              |
| 2:BT:79:GLU:HB3    | 2:BT:147:ALA:HB2   | 1.99                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 5:BW:67:ARG:NH2    | 16:Bi:228:PHE:O    | 2.42                     | 0.45              |
| 9:Bb:138:GLU:O     | 9:Bb:142:THR:HG22  | 2.17                     | 0.45              |
| 9:Bb:368:ARG:NH1   | 31:BA:1196:G:OP2   | 2.50                     | 0.45              |
| 10:Bc:294:GLN:HE22 | 10:Bc:320:VAL:H    | 1.65                     | 0.45              |
| 17:Bj:235:LYS:HE3  | 17:Bj:275:PHE:HD1  | 1.81                     | 0.45              |
| 19:Bl:141:ASN:ND2  | 31:BA:214:A:OP1    | 2.50                     | 0.45              |
| 21:Bn:123:ARG:NH1  | 31:BA:53:U:O2'     | 2.50                     | 0.45              |
| 27:Bv:37:PRO:HG3   | 27:Bv:64:HIS:CG    | 2.51                     | 0.45              |
| 29:Bw:265:LEU:N    | 29:Bw:266:PRO:HA   | 2.32                     | 0.45              |
| 31:AA:358:U:H2'    | 31:AA:359:U:C6     | 2.52                     | 0.45              |
| 31:AA:843:C:O2     | 31:AA:928:A:N6     | 2.50                     | 0.45              |
| 44:AR:125:TYR:HE2  | 45:AU:4:HIS:HB3    | 1.82                     | 0.45              |
| 56:Ag:158:HIS:HA   | 56:Ag:161:VAL:HG22 | 1.97                     | 0.45              |
| 65:FL:66:GLN:HA    | 65:FL:69:GLN:HG2   | 1.97                     | 0.45              |
| 65:FL:71:ILE:HA    | 65:FL:74:LEU:HG    | 1.99                     | 0.45              |
| 31:BA:97:A:H2'     | 31:BA:98:U:C6      | 2.52                     | 0.45              |
| 31:BA:122:G:N2     | 31:BA:125:A:OP2    | 2.49                     | 0.45              |
| 31:BA:481:A:H2'    | 31:BA:482:G:H8     | 1.82                     | 0.45              |
| 31:BA:722:A:H2'    | 31:BA:723:A:C8     | 2.52                     | 0.45              |
| 31:BA:1006:U:H2'   | 31:BA:1007:G:O4'   | 2.16                     | 0.45              |
| 31:BA:1173:A:H2'   | 31:BA:1174:C:C6    | 2.52                     | 0.45              |
| 31:BA:1569:A:N6    | 77:BE:153:SER:HA   | 2.31                     | 0.45              |
| 76:BD:113:ARG:O    | 76:BD:148:ARG:NH2  | 2.50                     | 0.45              |
| 8:Ba:283:TYR:CD1   | 8:Ba:284:PRO:HD2   | 2.52                     | 0.45              |
| 31:AA:552:A:H2'    | 31:AA:553:G:C8     | 2.52                     | 0.45              |
| 35:AF:9:ILE:HD12   | 35:AF:90:ARG:HB3   | 1.99                     | 0.45              |
| 38:AK:150:ARG:HG2  | 38:AK:175:ILE:HD11 | 1.99                     | 0.45              |
| 46:AV:9:C:H6       | 46:AV:42:A:H2'     | 1.81                     | 0.45              |
| 49:Aa:212:ASP:OD2  | 64:Ap:173:ARG:NH2  | 2.47                     | 0.45              |
| 53:Ae:222:SER:HA   | 53:Ae:225:VAL:HG22 | 1.99                     | 0.45              |
| 53:Ae:325:ARG:HH22 | 53:Ae:379:ARG:HH12 | 1.65                     | 0.45              |
| 63:Ao:520:LYS:O    | 63:Ao:527:ARG:NH2  | 2.50                     | 0.45              |
| 67:B3:66:LEU:HD12  | 67:B3:122:LEU:HD23 | 1.99                     | 0.45              |
| 73:B9:87:ILE:HB    | 73:B9:97:GLN:HB2   | 1.98                     | 0.45              |
| 31:BA:301:U:C2     | 31:BA:302:A:C8     | 3.05                     | 0.45              |
| 31:BA:1198:C:H2'   | 31:BA:1199:A:C8    | 2.52                     | 0.45              |
| 31:BA:1344:C:H2'   | 31:BA:1345:A:C8    | 2.51                     | 0.45              |
| 76:BD:181:ASP:HB3  | 76:BD:183:HIS:CE1  | 2.52                     | 0.45              |
| 77:BE:148:GLY:HA3  | 77:BE:173:LYS:HG3  | 1.99                     | 0.45              |
| 7:BY:65:LEU:HD11   | 7:BY:121:LYS:HG3   | 1.99                     | 0.44              |
| 10:Bc:313:LEU:O    | 10:Bc:317:ARG:HG2  | 2.17                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:AA:314:A:HO2'   | 31:AA:395:C:H41    | 1.55                     | 0.44              |
| 31:AA:512:A:H2'    | 31:AA:513:A:H8     | 1.82                     | 0.44              |
| 31:AA:619:C:P      | 33:AC:39:ALA:HA    | 2.56                     | 0.44              |
| 31:AA:836:G:H2'    | 31:AA:837:C:C6     | 2.52                     | 0.44              |
| 32:AB:117:LEU:HA   | 32:AB:120:THR:HB   | 1.99                     | 0.44              |
| 53:Ae:269:ALA:HB3  | 53:Ae:320:LEU:HD23 | 1.99                     | 0.44              |
| 55:Af:160:ASP:OD1  | 55:Af:160:ASP:N    | 2.49                     | 0.44              |
| 60:Ak:165:ILE:HG13 | 63:Ao:134:GLU:HB2  | 1.98                     | 0.44              |
| 64:Ap:136:HIS:NE2  | 64:Ap:139:TYR:HB2  | 2.33                     | 0.44              |
| 31:BA:181:C:H2'    | 31:BA:182:C:C6     | 2.52                     | 0.44              |
| 31:BA:232:U:H2'    | 31:BA:233:A:H8     | 1.83                     | 0.44              |
| 31:BA:306:A:H2'    | 31:BA:307:G:H8     | 1.82                     | 0.44              |
| 31:BA:378:U:OP2    | 84:BP:57:ARG:NH2   | 2.51                     | 0.44              |
| 31:BA:521:C:H2'    | 31:BA:522:A:H8     | 1.82                     | 0.44              |
| 31:BA:568:C:N3     | 82:BN:78:SER:HB2   | 2.32                     | 0.44              |
| 31:BA:815:A:H2'    | 31:BA:816:C:O4'    | 2.17                     | 0.44              |
| 75:BC:426:ALA:HB2  | 75:BC:431:PHE:HZ   | 1.81                     | 0.44              |
| 75:BC:617:HIS:CD2  | 75:BC:620:ASP:H    | 2.33                     | 0.44              |
| 94:BC:802:GNP:O1G  | 95:BC:901:HOH:O    | 2.21                     | 0.44              |
| 9:Bb:307:HIS:HB2   | 9:Bb:311:MET:HE2   | 1.99                     | 0.44              |
| 9:Bb:308:GLN:NE2   | 22:Bo:111:LYS:H    | 2.15                     | 0.44              |
| 26:Bu:94:VAL:HB    | 26:Bu:140:ARG:HH12 | 1.82                     | 0.44              |
| 31:AA:344:G:H1     | 38:AK:121:ASN:CG   | 2.25                     | 0.44              |
| 31:AA:419:A:H2'    | 31:AA:420:A:O4'    | 2.17                     | 0.44              |
| 31:AA:601:A:N6     | 58:Ai:63:GLY:HA3   | 2.32                     | 0.44              |
| 36:AG:69:LYS:HD3   | 36:AG:69:LYS:HA    | 1.82                     | 0.44              |
| 44:AR:96:HIS:CD2   | 44:AR:97:ILE:HG13  | 2.52                     | 0.44              |
| 64:Ap:116:ASP:OD1  | 64:Ap:117:PHE:N    | 2.50                     | 0.44              |
| 64:Ap:119:ASN:OD1  | 64:Ap:119:ASN:N    | 2.49                     | 0.44              |
| 65:LL:157:ASN:HB3  | 75:BC:259:ASN:ND2  | 2.32                     | 0.44              |
| 31:BA:53:U:H2'     | 31:BA:54:A:C8      | 2.51                     | 0.44              |
| 31:BA:363:G:H2'    | 31:BA:364:A:C8     | 2.53                     | 0.44              |
| 31:BA:373:U:H1'    | 31:BA:1146:G:O2'   | 2.17                     | 0.44              |
| 31:BA:415:A:H2'    | 31:BA:416:U:O4'    | 2.17                     | 0.44              |
| 31:BA:447:A:H61    | 85:BQ:140:MET:HE3  | 1.81                     | 0.44              |
| 31:BA:734:A:OP1    | 76:BD:103:ARG:N    | 2.37                     | 0.44              |
| 31:BA:1026:A:N3    | 31:BA:1278:C:O2'   | 2.46                     | 0.44              |
| 75:BC:59:LYS:N     | 94:BC:802:GNP:O1B  | 2.30                     | 0.44              |
| 77:BE:79:PRO:HG3   | 77:BE:192:PRO:HD2  | 1.98                     | 0.44              |
| 78:BF:71:GLY:HA3   | 78:BF:74:GLN:HE21  | 1.82                     | 0.44              |
| 81:BK:87:VAL:HG23  | 81:BK:124:LYS:HZ3  | 1.82                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AI:292:GLY:HA3   | 1:AI:325:GLY:HA2   | 1.99                     | 0.44              |
| 6:BX:25:PHE:CE1    | 66:B2:111:ARG:HD3  | 2.52                     | 0.44              |
| 9:Bb:214:TRP:HB3   | 9:Bb:272:LEU:HD11  | 1.98                     | 0.44              |
| 11:Bd:84:GLU:HA    | 11:Bd:87:MET:HG2   | 1.98                     | 0.44              |
| 12:Be:80:THR:O     | 66:B2:90:GLN:NE2   | 2.50                     | 0.44              |
| 31:AA:122:C:H4'    | 43:AQ:24:LYS:HD2   | 1.98                     | 0.44              |
| 31:AA:180:U:H2'    | 31:AA:181:A:C8     | 2.52                     | 0.44              |
| 31:AA:342:C:H2'    | 31:AA:343:U:C6     | 2.53                     | 0.44              |
| 31:AA:919:A:C4     | 75:BC:624:ILE:HG12 | 2.51                     | 0.44              |
| 46:AY:54:A:H2'     | 46:AY:55:C:H5''    | 1.99                     | 0.44              |
| 49:Aa:128:MET:HE2  | 49:Aa:132:GLN:HB3  | 1.98                     | 0.44              |
| 51:Ac:2:PRO:HB2    | 51:Ac:11:ARG:HH12  | 1.81                     | 0.44              |
| 60:Ak:68:TRP:HZ2   | 60:Ak:114:LEU:HD13 | 1.83                     | 0.44              |
| 61:Am:17:ARG:HH11  | 61:Am:20:ILE:HD11  | 1.80                     | 0.44              |
| 69:B5:156:THR:HG1  | 86:BR:130:CYS:HG   | 1.57                     | 0.44              |
| 31:BA:232:U:H2'    | 31:BA:233:A:C8     | 2.52                     | 0.44              |
| 31:BA:1303:C:H2'   | 31:BA:1304:G:O4'   | 2.17                     | 0.44              |
| 78:BF:283:LEU:HD11 | 84:BP:189:LYS:HE2  | 1.99                     | 0.44              |
| 83:BO:89:HIS:HA    | 83:BO:103:ASN:HD22 | 1.83                     | 0.44              |
| 9:Bb:217:LEU:HD11  | 9:Bb:233:VAL:HG12  | 2.00                     | 0.44              |
| 17:Bj:191:THR:HA   | 17:Bj:195:LEU:HD13 | 1.99                     | 0.44              |
| 30:Bx:84:GLU:HG3   | 82:BN:152:PRO:HB3  | 2.00                     | 0.44              |
| 31:AA:526:G:O2'    | 34:AE:232:THR:O    | 2.36                     | 0.44              |
| 31:AA:539:A:O2'    | 31:AA:788:G:OP2    | 2.24                     | 0.44              |
| 31:AA:681:A:H5''   | 34:AE:114:ARG:HH22 | 1.82                     | 0.44              |
| 48:AZ:703:ALA:HA   | 48:AZ:708:ALA:HB3  | 1.99                     | 0.44              |
| 53:Ae:227:TYR:CD1  | 53:Ae:394:LEU:HD11 | 2.52                     | 0.44              |
| 54:B1:41:VAL:HG21  | 54:B1:83:GLU:HB3   | 2.00                     | 0.44              |
| 56:Ag:275:ARG:HE   | 56:Ag:281:ILE:HG22 | 1.82                     | 0.44              |
| 62:An:189:TRP:NE1  | 62:An:191:THR:OG1  | 2.49                     | 0.44              |
| 31:BA:670:A:C6     | 31:BA:770:G:C6     | 3.06                     | 0.44              |
| 31:BA:790:A:N6     | 31:BA:1000:A:O2'   | 2.50                     | 0.44              |
| 75:BC:307:GLN:OE1  | 75:BC:307:GLN:N    | 2.46                     | 0.44              |
| 1:AI:277:ARG:HG3   | 1:AI:374:ASP:HB3   | 1.99                     | 0.44              |
| 6:BX:71:ARG:NH2    | 6:BX:73:GLN:OE1    | 2.46                     | 0.44              |
| 7:BY:214:TYR:HH    | 8:Ba:78:TRP:HE1    | 1.63                     | 0.44              |
| 8:Ba:133:PRO:HG3   | 8:Ba:375:TRP:CD2   | 2.52                     | 0.44              |
| 9:Bb:175:VAL:HG22  | 9:Bb:204:VAL:HG12  | 1.99                     | 0.44              |
| 10:Bc:99:LYS:HB3   | 10:Bc:99:LYS:HE2   | 1.77                     | 0.44              |
| 16:Bi:108:ARG:HE   | 16:Bi:215:ARG:HH11 | 1.65                     | 0.44              |
| 30:Bx:98:GLY:HA2   | 31:BA:1528:A:H2    | 1.82                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:AA:28:U:H2'     | 31:AA:29:A:C8      | 2.53                     | 0.44              |
| 31:AA:822:A:H3'    | 31:AA:823:G:C8     | 2.52                     | 0.44              |
| 31:AA:928:A:O2'    | 31:AA:929:A:H5'    | 2.17                     | 0.44              |
| 39:AL:93:CYS:SG    | 39:AL:94:PHE:N     | 2.91                     | 0.44              |
| 54:B1:96:LYS:NZ    | 31:BA:82:G:OP1     | 2.49                     | 0.44              |
| 56:Ag:67:TYR:OH    | 56:Ag:139:HIS:ND1  | 2.41                     | 0.44              |
| 31:BA:1448:A:H2'   | 31:BA:1449:U:H6    | 1.83                     | 0.44              |
| 75:BC:136:ARG:HB2  | 75:BC:165:TYR:CE2  | 2.52                     | 0.44              |
| 84:BP:44:ARG:HD3   | 84:BP:45:ARG:HG3   | 2.00                     | 0.44              |
| 12:Be:22:THR:OG1   | 12:Be:23:SER:N     | 2.51                     | 0.44              |
| 13:Bf:75:ILE:HG23  | 15:Bh:289:VAL:HG11 | 1.98                     | 0.44              |
| 16:Bi:164:VAL:O    | 16:Bi:260:ARG:NH2  | 2.42                     | 0.44              |
| 31:AA:368:A:H2'    | 31:AA:368:A:N3     | 2.32                     | 0.44              |
| 31:AA:938:U:H2'    | 31:AA:939:A:H8     | 1.81                     | 0.44              |
| 33:AC:53:TYR:O     | 33:AC:57:HIS:ND1   | 2.49                     | 0.44              |
| 56:Ag:205:GLU:HB3  | 56:Ag:207:TYR:CZ   | 2.52                     | 0.44              |
| 56:Ag:339:PHE:HE1  | 56:Ag:341:PRO:HB3  | 1.82                     | 0.44              |
| 31:BA:215:A:H61    | 31:BA:231:C:H42    | 1.66                     | 0.44              |
| 31:BA:620:A:H2'    | 31:BA:621:U:C6     | 2.52                     | 0.44              |
| 31:BA:1146:G:H2'   | 31:BA:1147:G:H8    | 1.82                     | 0.44              |
| 8:Ba:172:LYS:O     | 8:Ba:175:THR:OG1   | 2.25                     | 0.44              |
| 12:Be:25:ARG:HG2   | 31:BA:674:U:H5     | 1.82                     | 0.44              |
| 13:Bf:130:HIS:ND1  | 31:BA:172:C:O2'    | 2.43                     | 0.44              |
| 24:Bq:73:MET:SD    | 24:Bq:73:MET:N     | 2.86                     | 0.44              |
| 29:Bw:55:SER:HB2   | 31:BA:659:U:H5''   | 2.00                     | 0.44              |
| 29:Bw:99:ALA:HB3   | 29:Bw:102:ALA:HB2  | 2.00                     | 0.44              |
| 29:Bw:186:ASN:HD22 | 29:Bw:420:LEU:HA   | 1.82                     | 0.44              |
| 31:AA:34:U:O2      | 31:AA:223:U:O2'    | 2.36                     | 0.44              |
| 31:AA:75:A:N7      | 31:AA:146:U:O2     | 2.51                     | 0.44              |
| 31:AA:584:C:O2     | 40:AN:86:ARG:HG2   | 2.18                     | 0.44              |
| 33:AC:96:MET:HG3   | 33:AC:108:LEU:HD21 | 1.98                     | 0.44              |
| 36:AG:62:GLU:O     | 36:AG:66:ARG:NH1   | 2.50                     | 0.44              |
| 39:AL:109:LEU:HD22 | 39:AL:129:LYS:HE3  | 1.98                     | 0.44              |
| 56:Ag:328:LEU:HD13 | 56:Ag:336:LEU:HG   | 1.99                     | 0.44              |
| 59:Aj:41:MET:HE1   | 59:Aj:58:VAL:HG11  | 2.00                     | 0.44              |
| 73:B9:83:GLY:HA2   | 31:BA:1527:U:C6    | 2.52                     | 0.44              |
| 31:BA:119:A:C6     | 31:BA:120:C:C2     | 3.06                     | 0.44              |
| 31:BA:658:U:H2'    | 31:BA:659:U:H6     | 1.82                     | 0.44              |
| 31:BA:1065:G:H2'   | 31:BA:1066:A:C8    | 2.52                     | 0.44              |
| 75:BC:61:THR:O     | 75:BC:65:ARG:HG2   | 2.18                     | 0.44              |
| 80:BJ:56:PRO:HB3   | 85:BQ:210:GLN:HE21 | 1.83                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 83:BO:60:VAL:HG12  | 83:BO:62:ASN:H     | 1.83                     | 0.44              |
| 3:BU:116:LEU:HD21  | 4:BV:148:LEU:HD21  | 2.00                     | 0.44              |
| 9:Bb:138:GLU:HG2   | 9:Bb:141:ARG:HH22  | 1.83                     | 0.44              |
| 12:Be:129:TYR:CD1  | 66:B2:162:GLN:HG3  | 2.53                     | 0.44              |
| 17:Bj:248:LYS:HE3  | 17:Bj:250:GLY:HA3  | 2.00                     | 0.44              |
| 20:Bm:118:LEU:HB3  | 78:BF:63:GLN:HB2   | 2.00                     | 0.44              |
| 27:Bv:27:ALA:HB2   | 78:BF:243:VAL:HG12 | 1.98                     | 0.44              |
| 29:Bw:219:ARG:HH12 | 31:BA:779:G:H5''   | 1.83                     | 0.44              |
| 31:AA:144:C:H2'    | 31:AA:145:U:C6     | 2.52                     | 0.44              |
| 31:AA:245:C:H2'    | 31:AA:246:A:C8     | 2.53                     | 0.44              |
| 32:AB:116:ASP:OD2  | 32:AB:119:GLN:NE2  | 2.51                     | 0.44              |
| 35:AF:104:GLU:O    | 44:AR:103:LYS:NZ   | 2.39                     | 0.44              |
| 46:AV:24:U:H2'     | 46:AV:25:C:C6      | 2.53                     | 0.44              |
| 51:Ac:90:VAL:HG23  | 51:Ac:93:LYS:HB2   | 2.00                     | 0.44              |
| 53:Ae:163:ASP:OD1  | 53:Ae:163:ASP:N    | 2.50                     | 0.44              |
| 53:Ae:285:CYS:SG   | 53:Ae:286:ASN:N    | 2.91                     | 0.44              |
| 56:Ag:272:THR:HG23 | 56:Ag:315:LEU:HD23 | 1.99                     | 0.44              |
| 59:Aj:68:LEU:HD21  | 59:Aj:100:VAL:HG21 | 1.98                     | 0.44              |
| 60:Ak:66:GLN:HE22  | 63:Ao:83:THR:HG22  | 1.83                     | 0.44              |
| 63:Ao:433:GLU:H    | 63:Ao:433:GLU:CD   | 2.25                     | 0.44              |
| 31:BA:120:C:H2'    | 31:BA:121:C:C6     | 2.52                     | 0.44              |
| 31:BA:420:U:H2'    | 31:BA:421:U:C6     | 2.52                     | 0.44              |
| 31:BA:1234:U:O2'   | 84:BP:76:LEU:O     | 2.27                     | 0.44              |
| 75:BC:219:GLU:HG2  | 75:BC:276:ILE:HD13 | 2.00                     | 0.44              |
| 75:BC:490:GLU:OE2  | 75:BC:522:LYS:N    | 2.48                     | 0.44              |
| 75:BC:649:ILE:HD11 | 75:BC:721:GLN:HG2  | 2.00                     | 0.44              |
| 76:BD:83:GLY:HA2   | 76:BD:96:ILE:HG22  | 2.00                     | 0.44              |
| 84:BP:264:GLN:NE2  | 84:BP:269:LEU:O    | 2.51                     | 0.44              |
| 8:Ba:41:PRO:HG2    | 31:BA:42:C:N4      | 2.32                     | 0.44              |
| 9:Bb:304:TYR:CE2   | 9:Bb:313:PRO:HD3   | 2.53                     | 0.44              |
| 15:Bh:59:ARG:HA    | 15:Bh:184:PHE:CE1  | 2.53                     | 0.44              |
| 16:Bi:137:PHE:N    | 16:Bi:138:PRO:HD2  | 2.33                     | 0.44              |
| 17:Bj:55:ARG:HG3   | 17:Bj:238:LEU:HD23 | 2.00                     | 0.44              |
| 23:Bp:72:HIS:NE2   | 23:Bp:97:ARG:HD3   | 2.33                     | 0.44              |
| 28:B0:102:GLU:HB2  | 28:B0:130:PHE:CD2  | 2.52                     | 0.44              |
| 29:Bw:132:ASP:OD1  | 29:Bw:134:THR:OG1  | 2.21                     | 0.44              |
| 31:AA:411:U:H2'    | 31:AA:412:A:H8     | 1.83                     | 0.44              |
| 31:AA:548:G:N2     | 31:AA:785:U:O2     | 2.42                     | 0.44              |
| 31:AA:662:C:H2'    | 31:AA:663:A:H8     | 1.83                     | 0.44              |
| 31:AA:936:C:H2'    | 31:AA:937:A:H8     | 1.82                     | 0.44              |
| 51:Ac:90:VAL:HG21  | 51:Ac:98:ILE:HD11  | 2.00                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 54:B1:177:HIS:O    | 54:B1:184:ARG:NH2  | 2.51                     | 0.44              |
| 59:Aj:85:TRP:HH2   | 59:Aj:95:TRP:HE1   | 1.66                     | 0.44              |
| 66:B2:163:GLU:OE1  | 66:B2:163:GLU:N    | 2.51                     | 0.44              |
| 72:B8:94:VAL:HG21  | 72:B8:161:MET:HG2  | 2.00                     | 0.44              |
| 31:BA:635:U:H2'    | 31:BA:636:U:C6     | 2.52                     | 0.44              |
| 31:BA:913:G:H21    | 31:BA:914:A:N6     | 2.16                     | 0.44              |
| 31:BA:1140:A:H2'   | 31:BA:1141:A:C8    | 2.48                     | 0.44              |
| 31:BA:1344:C:C2    | 31:BA:1368:G:N2    | 2.86                     | 0.44              |
| 76:BD:186:GLY:HA2  | 76:BD:220:LYS:HD2  | 1.99                     | 0.44              |
| 9:Bb:235:TRP:HB2   | 9:Bb:254:TYR:HD1   | 1.83                     | 0.43              |
| 10:Bc:140:TRP:HZ3  | 86:BR:145:LEU:HD11 | 1.81                     | 0.43              |
| 10:Bc:312:LEU:HD13 | 86:BR:149:LEU:HD23 | 2.00                     | 0.43              |
| 16:Bi:170:PRO:HA   | 16:Bi:173:VAL:HG12 | 2.00                     | 0.43              |
| 26:Bu:119:ALA:O    | 26:Bu:123:LYS:HB3  | 2.18                     | 0.43              |
| 31:AA:167:G:OP1    | 83:BO:120:LYS:NZ   | 2.51                     | 0.43              |
| 31:AA:541:C:H2'    | 31:AA:542:C:C6     | 2.53                     | 0.43              |
| 31:AA:831:A:H2'    | 31:AA:832:G:H8     | 1.82                     | 0.43              |
| 42:AP:67:ALA:HB2   | 49:Aa:218:TYR:CZ   | 2.51                     | 0.43              |
| 53:Ae:80:TRP:HB2   | 53:Ae:154:ARG:HH11 | 1.83                     | 0.43              |
| 53:Ae:322:VAL:HA   | 53:Ae:325:ARG:HG2  | 2.00                     | 0.43              |
| 53:Ae:429:ARG:HE   | 53:Ae:433:ARG:HG3  | 1.81                     | 0.43              |
| 55:Af:144:ARG:HH12 | 55:Af:171:LEU:HD21 | 1.83                     | 0.43              |
| 63:Ao:656:PHE:HA   | 63:Ao:659:THR:HG22 | 1.99                     | 0.43              |
| 66:B2:153:ASP:HA   | 66:B2:156:ARG:HG2  | 1.99                     | 0.43              |
| 31:BA:181:C:H2'    | 31:BA:182:C:H6     | 1.83                     | 0.43              |
| 31:BA:368:A:O2'    | 31:BA:369:G:N7     | 2.51                     | 0.43              |
| 31:BA:453:U:C2     | 31:BA:454:U:C5     | 3.06                     | 0.43              |
| 31:BA:609:U:H2'    | 31:BA:610:C:C6     | 2.53                     | 0.43              |
| 31:BA:671:C:H2'    | 31:BA:672:G:C8     | 2.53                     | 0.43              |
| 31:BA:1020:C:H2'   | 31:BA:1021:C:H6    | 1.83                     | 0.43              |
| 31:BA:1236:C:H2'   | 31:BA:1237:A:C8    | 2.53                     | 0.43              |
| 75:BC:197:ASN:ND2  | 75:BC:256:CYS:O    | 2.46                     | 0.43              |
| 75:BC:386:ASN:OD1  | 75:BC:387:THR:N    | 2.51                     | 0.43              |
| 75:BC:530:THR:HG1  | 75:BC:642:THR:HG1  | 1.58                     | 0.43              |
| 76:BD:167:SER:HB3  | 76:BD:183:HIS:CD2  | 2.53                     | 0.43              |
| 77:BE:334:ASP:HB3  | 77:BE:337:VAL:HG23 | 2.00                     | 0.43              |
| 87:BS:68:TRP:C     | 87:BS:70:THR:H     | 2.26                     | 0.43              |
| 10:Bc:183:ASP:OD1  | 10:Bc:184:LYS:N    | 2.48                     | 0.43              |
| 31:AA:94:G:H2'     | 31:AA:95:A:H8      | 1.82                     | 0.43              |
| 31:AA:332:U:H2'    | 31:AA:333:A:C8     | 2.53                     | 0.43              |
| 31:AA:807:G:H2'    | 31:AA:809:G:C8     | 2.52                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 33:AC:87:VAL:HG21  | 58:Ai:53:PRO:HG2   | 2.01                     | 0.43              |
| 35:AF:92:ASN:CG    | 44:AR:118:LEU:HD22 | 2.43                     | 0.43              |
| 51:Ac:91:GLU:HG2   | 52:Ad:123:ARG:HH12 | 1.82                     | 0.43              |
| 53:Ae:147:TRP:CD1  | 53:Ae:147:TRP:H    | 2.37                     | 0.43              |
| 31:BA:119:A:C2     | 31:BA:120:C:H1'    | 2.53                     | 0.43              |
| 31:BA:322:G:C5     | 31:BA:341:G:C8     | 3.07                     | 0.43              |
| 31:BA:528:U:O2     | 31:BA:549:C:O2'    | 2.33                     | 0.43              |
| 75:BC:166:ASN:ND2  | 75:BC:166:ASN:O    | 2.51                     | 0.43              |
| 80:BJ:76:THR:HG23  | 80:BJ:79:VAL:H     | 1.83                     | 0.43              |
| 84:BP:178:PHE:HB2  | 84:BP:214:TYR:CE2  | 2.52                     | 0.43              |
| 1:AI:300:ASP:OD1   | 1:AI:301:TYR:N     | 2.52                     | 0.43              |
| 1:AI:302:LEU:HD22  | 56:Ag:384:ASN:HB3  | 2.00                     | 0.43              |
| 8:Ba:268:CYS:SG    | 8:Ba:269:ASN:N     | 2.90                     | 0.43              |
| 10:Bc:100:SER:HA   | 10:Bc:126:THR:HG22 | 2.00                     | 0.43              |
| 17:Bj:179:GLN:NE2  | 17:Bj:182:GLU:HB2  | 2.33                     | 0.43              |
| 46:AY:3:U:O4       | 46:AY:4:A:N6       | 2.51                     | 0.43              |
| 49:Aa:237:LEU:HG   | 49:Aa:241:TYR:CZ   | 2.52                     | 0.43              |
| 63:Ao:533:GLU:HA   | 63:Ao:536:MET:HE3  | 2.00                     | 0.43              |
| 65:GL:85:LEU:HD23  | 65:GL:88:LYS:HE2   | 2.01                     | 0.43              |
| 69:B5:79:ALA:HA    | 31:BA:1051:G:N2    | 2.33                     | 0.43              |
| 31:BA:13:U:H2'     | 31:BA:14:C:C6      | 2.53                     | 0.43              |
| 31:BA:230:G:H2'    | 31:BA:231:C:H6     | 1.84                     | 0.43              |
| 31:BA:248:A:H2'    | 31:BA:249:G:H8     | 1.82                     | 0.43              |
| 31:BA:1454:C:H2'   | 31:BA:1455:C:C6    | 2.53                     | 0.43              |
| 75:BC:559:LEU:HD12 | 75:BC:560:ASP:HB2  | 2.00                     | 0.43              |
| 78:BF:93:LEU:HD23  | 78:BF:96:LEU:HD12  | 2.00                     | 0.43              |
| 2:BT:161:GLU:OE1   | 2:BT:191:ARG:NH2   | 2.52                     | 0.43              |
| 5:BW:151:LEU:HB2   | 5:BW:167:LYS:HB2   | 2.00                     | 0.43              |
| 6:BX:144:VAL:HG21  | 16:Bi:276:ILE:HD12 | 2.00                     | 0.43              |
| 9:Bb:154:TYR:OH    | 87:BS:57:GLU:OE1   | 2.35                     | 0.43              |
| 12:Be:38:GLY:O     | 31:BA:37:A:N6      | 2.52                     | 0.43              |
| 22:Bo:74:ALA:HB2   | 67:B3:137:THR:HG21 | 2.00                     | 0.43              |
| 25:Bt:82:PHE:CG    | 25:Bt:83:PRO:HD2   | 2.53                     | 0.43              |
| 29:Bw:242:PRO:HD3  | 29:Bw:423:PRO:HA   | 2.00                     | 0.43              |
| 31:AA:108:G:H2'    | 31:AA:109:G:H8     | 1.83                     | 0.43              |
| 31:AA:182:A:C6     | 39:AL:56:PRO:HD2   | 2.53                     | 0.43              |
| 31:AA:364:U:H2'    | 31:AA:365:A:C8     | 2.53                     | 0.43              |
| 31:AA:829:G:H2'    | 31:AA:830:A:C8     | 2.53                     | 0.43              |
| 36:AG:158:LEU:HD21 | 36:AG:230:ALA:HA   | 2.00                     | 0.43              |
| 43:AQ:35:LEU:HB2   | 43:AQ:42:TYR:CE1   | 2.54                     | 0.43              |
| 53:Ae:125:ILE:HD11 | 53:Ae:155:GLN:HB3  | 2.00                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 58:Ai:6:GLU:HA     | 58:Ai:9:VAL:HG12   | 1.99                     | 0.43              |
| 67:B3:109:LYS:NZ   | 31:BA:417:G:N3     | 2.66                     | 0.43              |
| 31:BA:1238:A:H3'   | 31:BA:1239:A:H5''  | 2.00                     | 0.43              |
| 2:BT:98:ASP:OD2    | 77:BE:275:ARG:NH1  | 2.38                     | 0.43              |
| 4:BV:162:ALA:HB2   | 4:BV:199:ILE:HG13  | 2.00                     | 0.43              |
| 8:Ba:334:LYS:H     | 8:Ba:362:THR:HB    | 1.82                     | 0.43              |
| 15:Bh:83:PHE:HE2   | 15:Bh:202:LEU:HB2  | 1.82                     | 0.43              |
| 25:Bt:78:GLN:OE1   | 31:BA:391:A:N6     | 2.52                     | 0.43              |
| 31:AA:15:C:OP1     | 34:AE:339:SER:OG   | 2.22                     | 0.43              |
| 31:AA:235:A:H2'    | 31:AA:236:A:C4     | 2.54                     | 0.43              |
| 31:AA:262:C:H2'    | 31:AA:263:G:C8     | 2.53                     | 0.43              |
| 31:AA:365:A:H2'    | 31:AA:366:A:C8     | 2.53                     | 0.43              |
| 31:AA:397:U:H2'    | 31:AA:398:G:O4'    | 2.19                     | 0.43              |
| 31:AA:568:G:N2     | 37:AJ:126:ILE:HG21 | 2.34                     | 0.43              |
| 36:AG:157:GLY:HA3  | 36:AG:174:LEU:HD11 | 2.01                     | 0.43              |
| 38:AK:186:ASN:ND2  | 45:AU:42:ARG:HH22  | 2.17                     | 0.43              |
| 39:AL:57:GLN:HB3   | 39:AL:109:LEU:HD11 | 2.00                     | 0.43              |
| 53:Ae:137:HIS:C    | 59:Aj:104:TYR:HB2  | 2.43                     | 0.43              |
| 56:Ag:55:PRO:HA    | 56:Ag:58:HIS:CD2   | 2.53                     | 0.43              |
| 63:Ao:86:PRO:HG2   | 63:Ao:89:PHE:CD2   | 2.53                     | 0.43              |
| 31:BA:50:A:H8      | 31:BA:50:A:O5'     | 2.02                     | 0.43              |
| 31:BA:229:A:H1'    | 31:BA:230:G:C8     | 2.53                     | 0.43              |
| 31:BA:452:U:C2     | 31:BA:453:U:C5     | 3.06                     | 0.43              |
| 31:BA:1494:A:H2'   | 31:BA:1495:A:C8    | 2.53                     | 0.43              |
| 76:BD:76:PRO:HB2   | 76:BD:103:ARG:HD2  | 1.99                     | 0.43              |
| 79:BI:105:LEU:HD12 | 79:BI:112:VAL:HG21 | 2.00                     | 0.43              |
| 85:BQ:216:GLU:HG3  | 85:BQ:238:LYS:HE2  | 2.01                     | 0.43              |
| 87:BS:87:GLN:HG3   | 87:BS:88:HIS:CD2   | 2.54                     | 0.43              |
| 2:BT:275:THR:HG22  | 2:BT:278:ILE:HD12  | 2.00                     | 0.43              |
| 8:Ba:60:TYR:HB3    | 8:Ba:70:LEU:HD12   | 2.01                     | 0.43              |
| 9:Bb:304:TYR:HE2   | 9:Bb:313:PRO:HD3   | 1.81                     | 0.43              |
| 12:Be:44:ARG:NH1   | 29:Bw:158:PRO:HD3  | 2.34                     | 0.43              |
| 12:Be:129:TYR:HB3  | 12:Be:130:PRO:HD3  | 2.00                     | 0.43              |
| 22:Bo:34:ALA:HB2   | 22:Bo:40:TYR:CE2   | 2.53                     | 0.43              |
| 31:AA:67:C:H3'     | 31:AA:68:G:H8      | 1.82                     | 0.43              |
| 31:AA:914:A:H2'    | 31:AA:915:G:C8     | 2.53                     | 0.43              |
| 33:AC:89:ASP:O     | 33:AC:93:ARG:HG2   | 2.18                     | 0.43              |
| 40:AN:91:CYS:HB3   | 40:AN:96:ARG:H     | 1.83                     | 0.43              |
| 41:AO:141:GLU:O    | 41:AO:145:GLN:HG2  | 2.17                     | 0.43              |
| 65:LL:185:LYS:HD3  | 65:LL:197:LEU:HG   | 1.99                     | 0.43              |
| 31:BA:5:A:H2'      | 31:BA:6:A:C8       | 2.54                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:BA:199:A:H2'    | 31:BA:200:A:H8     | 1.84                     | 0.43              |
| 31:BA:1019:C:H2'   | 31:BA:1020:C:H6    | 1.82                     | 0.43              |
| 84:BP:251:GLU:HG3  | 84:BP:252:LEU:HG   | 2.01                     | 0.43              |
| 1:AI:119:LYS:HA    | 1:AI:122:ARG:HH11  | 1.83                     | 0.43              |
| 3:BU:145:VAL:HG21  | 22:Bo:31:GLN:NE2   | 2.33                     | 0.43              |
| 10:Bc:153:ARG:HH22 | 10:Bc:256:ASP:C    | 2.26                     | 0.43              |
| 16:Bi:251:HIS:HD2  | 16:Bi:254:ASP:HB2  | 1.84                     | 0.43              |
| 31:AA:489:G:H2'    | 31:AA:490:A:C8     | 2.53                     | 0.43              |
| 43:AQ:20:THR:HG21  | 43:AQ:59:THR:HA    | 2.00                     | 0.43              |
| 55:Af:131:ASP:HB3  | 55:Af:134:LYS:HD2  | 2.01                     | 0.43              |
| 56:Ag:47:ILE:HG13  | 56:Ag:65:GLN:HE22  | 1.84                     | 0.43              |
| 63:Ao:349:TYR:HD1  | 63:Ao:349:TYR:HA   | 1.71                     | 0.43              |
| 72:B8:113:ARG:HH21 | 84:BP:80:LYS:HE3   | 1.84                     | 0.43              |
| 72:B8:156:LYS:HE2  | 72:B8:156:LYS:HB3  | 1.83                     | 0.43              |
| 75:BC:535:PHE:CD1  | 75:BC:633:ALA:HB1  | 2.54                     | 0.43              |
| 78:BF:47:VAL:HG13  | 78:BF:78:GLY:HA3   | 2.01                     | 0.43              |
| 83:BO:128:ARG:HG2  | 83:BO:138:LEU:HD13 | 2.01                     | 0.43              |
| 1:AI:163:HIS:ND1   | 32:AB:155:GLU:OE1  | 2.52                     | 0.43              |
| 9:Bb:267:ARG:HD3   | 87:BS:52:ASN:HD22  | 1.83                     | 0.43              |
| 14:Bg:81:ASN:OD1   | 14:Bg:81:ASN:N     | 2.51                     | 0.43              |
| 31:AA:235:A:O2'    | 31:AA:236:A:O4'    | 2.33                     | 0.43              |
| 31:AA:580:U:O2'    | 31:AA:802:A:H1'    | 2.18                     | 0.43              |
| 31:AA:900:A:N3     | 31:AA:902:C:N4     | 2.67                     | 0.43              |
| 44:AR:86:SER:OG    | 44:AR:90:GLY:N     | 2.46                     | 0.43              |
| 72:B8:163:THR:HG22 | 72:B8:164:SER:H    | 1.83                     | 0.43              |
| 31:BA:199:A:H2'    | 31:BA:200:A:C8     | 2.54                     | 0.43              |
| 31:BA:1024:G:N1    | 31:BA:1028:A:OP2   | 2.43                     | 0.43              |
| 31:BA:1059:C:H2'   | 31:BA:1060:C:H6    | 1.84                     | 0.43              |
| 31:BA:1390:G:H2'   | 31:BA:1391:U:C6    | 2.54                     | 0.43              |
| 85:BQ:81:GLU:OE2   | 85:BQ:199:ARG:NH1  | 2.43                     | 0.43              |
| 1:AI:85:LYS:NZ     | 1:AI:99:PHE:O      | 2.42                     | 0.43              |
| 2:BT:192:ASP:CG    | 2:BT:230:SER:H     | 2.27                     | 0.43              |
| 3:BU:71:ARG:NH1    | 5:BW:208:HIS:O     | 2.46                     | 0.43              |
| 3:BU:126:GLU:HG2   | 4:BV:70:LEU:HD21   | 1.99                     | 0.43              |
| 6:BX:2:ALA:N       | 6:BX:7:TYR:OH      | 2.49                     | 0.43              |
| 9:Bb:308:GLN:HE22  | 22:Bo:111:LYS:H    | 1.65                     | 0.43              |
| 11:Bd:106:LEU:HG   | 17:Bj:212:HIS:HE1  | 1.83                     | 0.43              |
| 11:Bd:113:LEU:HA   | 11:Bd:116:GLU:HG2  | 2.00                     | 0.43              |
| 27:Bv:30:PRO:HA    | 27:Bv:31:PRO:HD3   | 1.95                     | 0.43              |
| 27:Bv:128:MET:HA   | 27:Bv:128:MET:HE3  | 2.01                     | 0.43              |
| 29:Bw:202:PHE:O    | 29:Bw:226:GLN:NE2  | 2.52                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:AA:131:U:O4     | 31:AA:132:A:N6     | 2.52                     | 0.43              |
| 31:AA:738:U:H3'    | 36:AG:198:ARG:HH21 | 1.84                     | 0.43              |
| 31:AA:815:U:H2'    | 31:AA:816:U:C6     | 2.54                     | 0.43              |
| 61:Am:99:LEU:HD21  | 61:Am:104:LEU:HD21 | 2.00                     | 0.43              |
| 65:DL:86:LEU:HD21  | 80:BJ:207:LEU:HD12 | 2.01                     | 0.43              |
| 72:B8:118:HIS:CD2  | 72:B8:169:ARG:HD3  | 2.53                     | 0.43              |
| 31:BA:562:A:H3'    | 31:BA:562:A:N3     | 2.34                     | 0.43              |
| 31:BA:1551:C:C5    | 77:BE:158:SER:HB3  | 2.54                     | 0.43              |
| 75:BC:284:ARG:O    | 75:BC:288:LEU:HG   | 2.19                     | 0.43              |
| 76:BD:168:ASP:HA   | 76:BD:184:PRO:HD3  | 2.00                     | 0.43              |
| 84:BP:97:SER:HB2   | 84:BP:143:GLU:HB3  | 2.01                     | 0.43              |
| 1:AI:159:TYR:CD1   | 32:AB:168:ARG:HG3  | 2.54                     | 0.43              |
| 8:Ba:240:ALA:HB2   | 8:Ba:375:TRP:HH2   | 1.84                     | 0.43              |
| 10:Bc:141:ARG:NH1  | 10:Bc:263:GLY:HA3  | 2.34                     | 0.43              |
| 11:Bd:105:GLU:HG3  | 17:Bj:214:LYS:HE2  | 2.01                     | 0.43              |
| 30:Bx:60:SER:HB2   | 30:Bx:75:TRP:HH2   | 1.84                     | 0.43              |
| 31:AA:765:A:C8     | 31:AA:767:U:C4     | 3.06                     | 0.43              |
| 31:AA:767:U:C2     | 31:AA:768:A:C8     | 3.07                     | 0.43              |
| 33:AC:154:HIS:CD2  | 60:Ak:77:PRO:HG3   | 2.54                     | 0.43              |
| 49:Aa:221:ARG:HH12 | 49:Aa:224:ARG:HE   | 1.66                     | 0.43              |
| 53:Ae:216:PRO:O    | 53:Ae:219:GLN:NE2  | 2.49                     | 0.43              |
| 56:Ag:89:GLN:HE21  | 56:Ag:93:PHE:HE2   | 1.65                     | 0.43              |
| 59:Aj:88:GLN:HA    | 64:Ap:215:ARG:HD3  | 2.01                     | 0.43              |
| 63:Ao:145:PHE:HA   | 63:Ao:163:LEU:HD13 | 2.00                     | 0.43              |
| 63:Ao:431:ASP:HB3  | 63:Ao:434:LEU:HD12 | 2.00                     | 0.43              |
| 63:Ao:586:PHE:HA   | 63:Ao:589:ALA:HB3  | 2.01                     | 0.43              |
| 65:CL:63:LYS:NZ    | 65:DL:70:ASP:HB3   | 2.34                     | 0.43              |
| 31:BA:123:U:H1'    | 31:BA:254:G:C6     | 2.54                     | 0.43              |
| 31:BA:276:G:O2'    | 31:BA:310:G:H4'    | 2.19                     | 0.43              |
| 31:BA:622:A:N6     | 31:BA:623:G:O6     | 2.52                     | 0.43              |
| 31:BA:1021:C:H2'   | 31:BA:1022:G:H8    | 1.82                     | 0.43              |
| 81:BK:17:SER:HB2   | 81:BK:72:VAL:HB    | 2.00                     | 0.43              |
| 82:BN:136:ASP:OD1  | 82:BN:136:ASP:N    | 2.52                     | 0.43              |
| 83:BO:41:VAL:HG12  | 83:BO:105:VAL:O    | 2.19                     | 0.43              |
| 84:BP:191:VAL:HB   | 84:BP:192:PRO:HD3  | 2.01                     | 0.43              |
| 1:AI:276:LYS:HA    | 1:AI:280:ALA:O     | 2.18                     | 0.42              |
| 3:BU:112:THR:H     | 14:Bg:127:GLN:NE2  | 2.17                     | 0.42              |
| 14:Bg:2:THR:HG22   | 14:Bg:5:GLY:H      | 1.84                     | 0.42              |
| 16:Bi:289:PRO:HG2  | 16:Bi:290:TRP:CE3  | 2.54                     | 0.42              |
| 20:Bm:61:TYR:HD1   | 20:Bm:134:PRO:HA   | 1.84                     | 0.42              |
| 26:Bu:118:LEU:HD11 | 26:Bu:157:ILE:HD13 | 2.01                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 30:Bx:146:ARG:HH21 | 31:BA:1531:C:P     | 2.42                     | 0.42              |
| 31:AA:155:A:H2'    | 31:AA:156:C:C6     | 2.54                     | 0.42              |
| 34:AE:289:THR:HG21 | 34:AE:308:GLN:H    | 1.84                     | 0.42              |
| 53:Ae:88:CYS:SG    | 53:Ae:89:HIS:N     | 2.92                     | 0.42              |
| 31:BA:370:A:H1'    | 31:BA:1201:A:N7    | 2.34                     | 0.42              |
| 31:BA:1301:A:H1'   | 31:BA:1351:U:O2'   | 2.19                     | 0.42              |
| 31:BA:1381:A:H2'   | 31:BA:1382:C:C6    | 2.54                     | 0.42              |
| 75:BC:170:LEU:HG   | 75:BC:317:LEU:HD21 | 2.01                     | 0.42              |
| 75:BC:600:SER:OG   | 75:BC:602:HIS:ND1  | 2.52                     | 0.42              |
| 76:BD:186:GLY:O    | 76:BD:220:LYS:NZ   | 2.42                     | 0.42              |
| 6:BX:71:ARG:HE     | 31:BA:704:U:H2'    | 1.84                     | 0.42              |
| 8:Ba:51:GLU:HB3    | 54:B1:123:PHE:HE1  | 1.84                     | 0.42              |
| 8:Ba:373:LEU:HD12  | 8:Ba:373:LEU:HA    | 1.89                     | 0.42              |
| 10:Bc:244:ASN:CG   | 10:Bc:248:ILE:H    | 2.27                     | 0.42              |
| 16:Bi:194:VAL:HG22 | 16:Bi:214:VAL:HG22 | 2.01                     | 0.42              |
| 17:Bj:277:LEU:HD11 | 18:Bk:172:GLU:HG3  | 2.01                     | 0.42              |
| 25:Bt:16:GLN:HB3   | 25:Bt:17:TRP:CD1   | 2.54                     | 0.42              |
| 31:AA:61:G:N2      | 31:AA:198:C:O3'    | 2.52                     | 0.42              |
| 31:AA:930:G:OP1    | 31:AA:933:A:H4'    | 2.19                     | 0.42              |
| 31:AA:940:C:H2'    | 31:AA:941:U:C6     | 2.54                     | 0.42              |
| 42:AP:100:HIS:ND1  | 42:AP:101:PRO:HD2  | 2.34                     | 0.42              |
| 43:AQ:13:VAL:O     | 43:AQ:65:LEU:HD12  | 2.19                     | 0.42              |
| 54:B1:176:LEU:HD23 | 54:B1:184:ARG:HG3  | 2.01                     | 0.42              |
| 56:Ag:204:GLN:HE21 | 56:Ag:249:GLN:HG2  | 1.83                     | 0.42              |
| 56:Ag:289:ILE:O    | 56:Ag:293:ARG:HG3  | 2.19                     | 0.42              |
| 59:Aj:85:TRP:HA    | 59:Aj:89:HIS:HD2   | 1.84                     | 0.42              |
| 71:B7:69:TRP:CE2   | 31:BA:34:A:C2      | 3.08                     | 0.42              |
| 31:BA:339:G:N3     | 31:BA:1067:G:O2'   | 2.47                     | 0.42              |
| 31:BA:1146:G:H2'   | 31:BA:1147:G:C8    | 2.54                     | 0.42              |
| 31:BA:1552:C:H5'   | 31:BA:1553:A:OP1   | 2.19                     | 0.42              |
| 74:BB:9:A:H8       | 74:BB:11:C:H41     | 1.67                     | 0.42              |
| 74:BB:28:A:N6      | 74:BB:29:G:O6      | 2.52                     | 0.42              |
| 75:BC:624:ILE:H    | 75:BC:624:ILE:HG13 | 1.52                     | 0.42              |
| 4:BV:181:ARG:NH2   | 31:BA:188:C:H3'    | 2.34                     | 0.42              |
| 6:BX:69:ARG:HH22   | 6:BX:98:GLN:HE21   | 1.67                     | 0.42              |
| 7:BY:22:GLY:HA3    | 7:BY:34:LYS:HZ3    | 1.85                     | 0.42              |
| 8:Ba:43:PRO:HA     | 8:Ba:44:PRO:HD3    | 1.94                     | 0.42              |
| 8:Ba:115:GLU:H     | 8:Ba:119:GLN:NE2   | 2.17                     | 0.42              |
| 9:Bb:130:ILE:H     | 87:BS:130:ARG:HH22 | 1.66                     | 0.42              |
| 11:Bd:43:ASP:HB3   | 68:B4:46:ARG:HH22  | 1.84                     | 0.42              |
| 20:Bm:74:HIS:HA    | 20:Bm:77:GLU:HG2   | 2.00                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:AA:96:U:H2'     | 31:AA:97:C:H6      | 1.84                     | 0.42              |
| 31:AA:434:A:H2'    | 31:AA:435:C:C6     | 2.54                     | 0.42              |
| 31:AA:523:C:H2'    | 31:AA:524:U:C6     | 2.55                     | 0.42              |
| 31:AA:532:G:C6     | 31:AA:834:A:C6     | 3.07                     | 0.42              |
| 31:AA:602:A:H2'    | 31:AA:603:U:C6     | 2.54                     | 0.42              |
| 42:AP:49:GLU:OE1   | 42:AP:76:TRP:NE1   | 2.48                     | 0.42              |
| 56:Ag:383:SER:HB2  | 56:Ag:389:GLN:HB3  | 2.02                     | 0.42              |
| 70:B6:20:MET:HG2   | 70:B6:58:GLU:HA    | 2.00                     | 0.42              |
| 31:BA:805:C:H2'    | 31:BA:806:U:O4'    | 2.19                     | 0.42              |
| 31:BA:806:U:H1'    | 77:BE:231:HIS:CE1  | 2.54                     | 0.42              |
| 75:BC:679:ASP:OD1  | 75:BC:679:ASP:N    | 2.47                     | 0.42              |
| 83:BO:43:ASN:OD1   | 83:BO:43:ASN:N     | 2.51                     | 0.42              |
| 6:BX:131:GLN:HA    | 6:BX:134:LYS:HG2   | 2.01                     | 0.42              |
| 8:Ba:387:TRP:HE1   | 8:Ba:404:ILE:HD12  | 1.84                     | 0.42              |
| 9:Bb:261:ARG:HH21  | 9:Bb:341:VAL:HG11  | 1.84                     | 0.42              |
| 12:Be:82:THR:H     | 66:B2:90:GLN:NE2   | 2.18                     | 0.42              |
| 20:Bm:137:ASP:OD2  | 78:BF:211:ARG:NH1  | 2.50                     | 0.42              |
| 31:AA:69:G:H2'     | 31:AA:70:U:H6      | 1.83                     | 0.42              |
| 31:AA:180:U:O4     | 31:AA:181:A:N6     | 2.53                     | 0.42              |
| 31:AA:549:A:C6     | 31:AA:550:G:C6     | 3.07                     | 0.42              |
| 46:AY:56:C:H2'     | 46:AY:57:C:C6      | 2.54                     | 0.42              |
| 56:Ag:158:HIS:ND1  | 56:Ag:313:GLY:O    | 2.52                     | 0.42              |
| 56:Ag:191:LYS:HE3  | 56:Ag:226:GLU:HG2  | 2.01                     | 0.42              |
| 63:Ao:92:ASP:O     | 63:Ao:96:ILE:HG13  | 2.19                     | 0.42              |
| 71:B7:74:ARG:HD3   | 71:B7:74:ARG:HA    | 1.83                     | 0.42              |
| 31:BA:189:A:N6     | 31:BA:1024:G:H21   | 2.16                     | 0.42              |
| 31:BA:636:U:O4     | 31:BA:637:A:N6     | 2.53                     | 0.42              |
| 31:BA:654:G:N1     | 31:BA:657:U:N3     | 2.67                     | 0.42              |
| 31:BA:1060:C:H5''  | 31:BA:1152:G:O2'   | 2.20                     | 0.42              |
| 31:BA:1336:A:C6    | 31:BA:1397:G:C6    | 3.08                     | 0.42              |
| 31:BA:1459:U:H3    | 31:BA:1468:A:H8    | 1.63                     | 0.42              |
| 75:BC:191:ARG:NH1  | 75:BC:198:ALA:O    | 2.48                     | 0.42              |
| 75:BC:359:LYS:HB3  | 75:BC:370:TYR:HB2  | 2.02                     | 0.42              |
| 75:BC:360:LEU:HD22 | 75:BC:367:GLN:HE22 | 1.84                     | 0.42              |
| 81:BK:140:VAL:O    | 81:BK:144:ILE:HG12 | 2.19                     | 0.42              |
| 84:BP:211:VAL:O    | 84:BP:215:THR:OG1  | 2.26                     | 0.42              |
| 6:BX:71:ARG:NH2    | 31:BA:703:A:O2'    | 2.52                     | 0.42              |
| 9:Bb:151:LEU:HD21  | 87:BS:103:VAL:HG13 | 2.02                     | 0.42              |
| 12:Be:25:ARG:HG2   | 31:BA:674:U:C5     | 2.54                     | 0.42              |
| 24:Bq:136:ARG:NH2  | 31:BA:546:C:O2'    | 2.52                     | 0.42              |
| 29:Bw:95:PRO:HG2   | 29:Bw:229:ASP:HB2  | 2.01                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:AA:110:U:O2'    | 31:AA:113:C:OP1    | 2.34                     | 0.42              |
| 31:AA:250:A:H2'    | 31:AA:251:C:C6     | 2.55                     | 0.42              |
| 31:AA:530:G:H21    | 31:AA:931:G:H2'    | 1.84                     | 0.42              |
| 31:AA:604:U:H1'    | 58:Ai:95:ARG:HD3   | 2.01                     | 0.42              |
| 31:AA:606:A:H3'    | 31:AA:607:G:C8     | 2.55                     | 0.42              |
| 34:AE:140:LEU:HD21 | 34:AE:160:ARG:NE   | 2.33                     | 0.42              |
| 39:AL:129:LYS:HD3  | 39:AL:129:LYS:HA   | 1.72                     | 0.42              |
| 42:AP:19:ILE:HG12  | 42:AP:36:ALA:HB2   | 2.01                     | 0.42              |
| 61:Am:52:MET:HG3   | 61:Am:70:ILE:HD13  | 2.02                     | 0.42              |
| 64:Ap:68:TYR:HE2   | 64:Ap:109:ARG:HH21 | 1.68                     | 0.42              |
| 31:BA:175:C:O2'    | 82:BN:49:GLN:HB3   | 2.19                     | 0.42              |
| 31:BA:429:G:O2'    | 31:BA:599:A:N3     | 2.41                     | 0.42              |
| 31:BA:1569:A:H5'   | 77:BE:62:LYS:HE2   | 2.00                     | 0.42              |
| 75:BC:549:TYR:CD1  | 75:BC:617:HIS:HB2  | 2.54                     | 0.42              |
| 84:BP:177:ALA:HA   | 84:BP:222:TYR:CD1  | 2.53                     | 0.42              |
| 84:BP:255:MET:HE3  | 84:BP:255:MET:HB3  | 1.97                     | 0.42              |
| 3:BU:149:ARG:HD2   | 13:Bf:56:ARG:HD3   | 2.00                     | 0.42              |
| 4:BV:179:GLN:HG2   | 4:BV:182:LYS:HD2   | 2.01                     | 0.42              |
| 8:Ba:332:ASP:OD1   | 8:Ba:333:SER:N     | 2.53                     | 0.42              |
| 9:Bb:70:TRP:CD1    | 9:Bb:70:TRP:H      | 2.37                     | 0.42              |
| 10:Bc:183:ASP:HB3  | 10:Bc:186:LEU:HD13 | 2.02                     | 0.42              |
| 15:Bh:105:ARG:HB2  | 15:Bh:112:LYS:HD2  | 2.01                     | 0.42              |
| 15:Bh:240:LEU:HD23 | 15:Bh:301:LEU:HD21 | 2.02                     | 0.42              |
| 29:Bw:195:ASP:OD2  | 29:Bw:236:ARG:NE   | 2.43                     | 0.42              |
| 31:AA:236:A:N3     | 31:AA:269:C:H1'    | 2.35                     | 0.42              |
| 31:AA:539:A:H8     | 31:AA:788:G:H3'    | 1.85                     | 0.42              |
| 31:AA:562:A:H1'    | 31:AA:708:A:H61    | 1.84                     | 0.42              |
| 43:AQ:95:VAL:HG12  | 51:Ac:87:LEU:HD21  | 2.00                     | 0.42              |
| 45:AU:83:PRO:HG2   | 45:AU:84:TRP:CD1   | 2.55                     | 0.42              |
| 46:AV:1:A:H2'      | 46:AV:2:G:C8       | 2.54                     | 0.42              |
| 48:AZ:698:ALA:HB1  | 48:AZ:701:ALA:HB3  | 2.00                     | 0.42              |
| 54:B1:10:LEU:HG    | 31:BA:68:A:N6      | 2.34                     | 0.42              |
| 31:BA:1155:G:C6    | 31:BA:1156:A:C5    | 3.08                     | 0.42              |
| 8:Ba:185:ILE:HD11  | 8:Ba:292:TYR:CE2   | 2.54                     | 0.42              |
| 13:Bf:67:ILE:HG21  | 15:Bh:258:THR:HG23 | 2.01                     | 0.42              |
| 23:Bp:43:ARG:HH12  | 80:BJ:104:LEU:HB2  | 1.84                     | 0.42              |
| 25:Bt:15:ARG:HG2   | 25:Bt:16:GLN:H     | 1.84                     | 0.42              |
| 29:Bw:198:ARG:HG3  | 29:Bw:199:PRO:HD2  | 2.01                     | 0.42              |
| 31:AA:342:C:OP1    | 38:AK:96:ASN:ND2   | 2.53                     | 0.42              |
| 31:AA:397:U:H5''   | 31:AA:462:A:O2'    | 2.20                     | 0.42              |
| 31:AA:956:G:H2'    | 31:AA:957:A:C8     | 2.55                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 33:AC:101:PRO:HG2  | 58:Ai:72:ARG:HH21  | 1.85                     | 0.42              |
| 34:AE:130:GLN:O    | 58:Ai:72:ARG:NH1   | 2.53                     | 0.42              |
| 37:AJ:76:LEU:HB3   | 37:AJ:145:LEU:HB2  | 2.02                     | 0.42              |
| 42:AP:21:LEU:HB3   | 42:AP:32:TYR:HB3   | 2.02                     | 0.42              |
| 53:Ae:281:ARG:HA   | 53:Ae:284:TYR:CZ   | 2.54                     | 0.42              |
| 61:Am:66:CYS:SG    | 61:Am:69:GLU:HB2   | 2.60                     | 0.42              |
| 63:Ao:489:PHE:HD1  | 63:Ao:489:PHE:HA   | 1.76                     | 0.42              |
| 64:Ap:108:CYS:SG   | 64:Ap:146:GLN:HG3  | 2.60                     | 0.42              |
| 31:BA:449:C:H2'    | 31:BA:450:U:H6     | 1.84                     | 0.42              |
| 31:BA:654:G:N1     | 31:BA:657:U:C2     | 2.88                     | 0.42              |
| 74:BB:30:G:H2'     | 74:BB:31:C:C6      | 2.55                     | 0.42              |
| 79:BI:87:LYS:HG3   | 79:BI:88:HIS:CD2   | 2.54                     | 0.42              |
| 4:BV:181:ARG:HH21  | 31:BA:188:C:P      | 2.43                     | 0.42              |
| 8:Ba:201:ARG:HG2   | 8:Ba:232:ALA:HB2   | 2.02                     | 0.42              |
| 8:Ba:322:LEU:HD23  | 8:Ba:322:LEU:HA    | 1.88                     | 0.42              |
| 9:Bb:120:GLU:OE2   | 9:Bb:124:ARG:NH2   | 2.53                     | 0.42              |
| 15:Bh:269:VAL:HG22 | 82:BN:11:TRP:NE1   | 2.35                     | 0.42              |
| 16:Bi:56:PHE:HD1   | 16:Bi:56:PHE:HA    | 1.76                     | 0.42              |
| 31:AA:181:A:O2'    | 31:AA:183:A:N7     | 2.43                     | 0.42              |
| 31:AA:923:G:H1'    | 31:AA:944:A:H2     | 1.85                     | 0.42              |
| 34:AE:425:LEU:HD13 | 64:Ap:85:ILE:HG21  | 2.02                     | 0.42              |
| 38:AK:90:ILE:HG12  | 38:AK:99:ILE:HG12  | 2.01                     | 0.42              |
| 46:AV:24:U:H2'     | 46:AV:25:C:H6      | 1.83                     | 0.42              |
| 49:Aa:272:TYR:HA   | 49:Aa:275:ILE:HG12 | 2.01                     | 0.42              |
| 53:Ae:178:PHE:CG   | 59:Aj:72:PRO:HA    | 2.54                     | 0.42              |
| 55:Af:109:VAL:HG12 | 55:Af:110:GLU:H    | 1.84                     | 0.42              |
| 64:Ap:105:CYS:HB3  | 64:Ap:142:VAL:HA   | 2.02                     | 0.42              |
| 65:LL:164:LEU:HG   | 65:LL:170:GLN:HG2  | 2.01                     | 0.42              |
| 31:BA:215:A:N6     | 31:BA:231:C:H42    | 2.18                     | 0.42              |
| 31:BA:580:A:H2'    | 31:BA:581:A:O4'    | 2.20                     | 0.42              |
| 78:BF:83:HIS:CG    | 78:BF:274:LEU:HD11 | 2.55                     | 0.42              |
| 1:AI:177:ASN:HA    | 1:AI:180:ARG:HE    | 1.85                     | 0.42              |
| 9:Bb:304:TYR:O     | 9:Bb:308:GLN:HB2   | 2.20                     | 0.42              |
| 14:Bg:2:THR:HG23   | 31:BA:166:A:H5''   | 2.01                     | 0.42              |
| 15:Bh:188:PRO:N    | 15:Bh:189:PRO:HD2  | 2.34                     | 0.42              |
| 23:Bp:17:ARG:HE    | 23:Bp:65:ASP:HB2   | 1.85                     | 0.42              |
| 28:B0:59:HIS:NE2   | 31:BA:412:C:O2'    | 2.42                     | 0.42              |
| 28:B0:78:GLY:HA2   | 87:BS:68:TRP:CE3   | 2.54                     | 0.42              |
| 31:AA:192:C:H2'    | 31:AA:193:A:H8     | 1.83                     | 0.42              |
| 40:AN:74:GLU:O     | 40:AN:77:SER:OG    | 2.35                     | 0.42              |
| 56:Ag:135:LEU:HD13 | 56:Ag:135:LEU:HA   | 1.94                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 60:Ak:214:CYS:O    | 60:Ak:220:ASN:ND2  | 2.42                     | 0.42              |
| 65:HL:76:LEU:HA    | 65:HL:79:ILE:HG22  | 2.02                     | 0.42              |
| 65:LL:144:LYS:HG2  | 65:LL:191:VAL:HB   | 2.01                     | 0.42              |
| 31:BA:188:C:O2'    | 31:BA:190:U:OP2    | 2.26                     | 0.42              |
| 31:BA:860:G:H2'    | 31:BA:860:G:N3     | 2.34                     | 0.42              |
| 31:BA:937:C:H3'    | 31:BA:938:U:H5''   | 2.02                     | 0.42              |
| 31:BA:1294:A:H3'   | 31:BA:1295:G:H8    | 1.85                     | 0.42              |
| 31:BA:1315:U:H2'   | 31:BA:1316:U:C6    | 2.55                     | 0.42              |
| 31:BA:1404:G:OP2   | 31:BA:1404:G:N2    | 2.22                     | 0.42              |
| 87:BS:52:ASN:OD1   | 87:BS:55:ASN:N     | 2.53                     | 0.42              |
| 7:BY:133:VAL:HG11  | 7:BY:145:ARG:HD2   | 2.02                     | 0.42              |
| 8:Ba:48:ARG:HB3    | 54:B1:157:PHE:HD2  | 1.85                     | 0.42              |
| 8:Ba:203:CYS:H     | 29:Bw:173:GLN:NE2  | 2.17                     | 0.42              |
| 9:Bb:35:MET:HB2    | 9:Bb:38:GLU:HB3    | 2.02                     | 0.42              |
| 14:Bg:28:ARG:NH1   | 15:Bh:71:GLU:OE2   | 2.43                     | 0.42              |
| 24:Bq:111:ASP:OD2  | 24:Bq:113:GLU:HB2  | 2.19                     | 0.42              |
| 29:Bw:298:ASP:HA   | 29:Bw:301:LYS:HE3  | 2.02                     | 0.42              |
| 30:Bx:107:LEU:HD13 | 30:Bx:115:ILE:HD12 | 2.01                     | 0.42              |
| 31:AA:9:U:H1'      | 31:AA:518:A:H5''   | 2.01                     | 0.42              |
| 31:AA:204:U:H2'    | 31:AA:205:U:C6     | 2.55                     | 0.42              |
| 31:AA:533:C:H2'    | 31:AA:534:U:H6     | 1.85                     | 0.42              |
| 31:AA:572:A:OP2    | 31:AA:573:A:O2'    | 2.34                     | 0.42              |
| 34:AE:213:GLU:CD   | 34:AE:213:GLU:H    | 2.27                     | 0.42              |
| 37:AJ:106:ILE:HD11 | 37:AJ:143:LEU:HB3  | 2.02                     | 0.42              |
| 46:AY:26:G:H2'     | 46:AY:27:G:O4'     | 2.20                     | 0.42              |
| 49:Aa:89:LYS:HD3   | 49:Aa:90:PRO:HD2   | 2.02                     | 0.42              |
| 56:Ag:66:HIS:NE2   | 56:Ag:99:MET:HB2   | 2.35                     | 0.42              |
| 63:Ao:500:LEU:HD11 | 63:Ao:534:ILE:HG22 | 2.02                     | 0.42              |
| 65:DL:77:LEU:HD11  | 80:BJ:186:LEU:HD11 | 2.01                     | 0.42              |
| 68:B4:47:GLN:NE2   | 74:BB:34:U:OP1     | 2.53                     | 0.42              |
| 31:BA:75:A:N1      | 31:BA:89:A:H5''    | 2.34                     | 0.42              |
| 31:BA:1136:U:O4    | 31:BA:1137:A:N6    | 2.53                     | 0.42              |
| 75:BC:220:GLU:C    | 75:BC:238:ILE:HD11 | 2.45                     | 0.42              |
| 75:BC:551:LYS:HB3  | 75:BC:615:ALA:HB3  | 2.02                     | 0.42              |
| 83:BO:69:VAL:HG23  | 83:BO:89:HIS:CE1   | 2.55                     | 0.42              |
| 85:BQ:72:ILE:HD11  | 85:BQ:96:TYR:CE1   | 2.55                     | 0.42              |
| 1:AI:277:ARG:NH2   | 31:AA:791:G:O6     | 2.53                     | 0.41              |
| 2:BT:237:LYS:HA    | 31:BA:1491:A:N1    | 2.35                     | 0.41              |
| 9:Bb:175:VAL:HB    | 9:Bb:187:VAL:HB    | 2.02                     | 0.41              |
| 9:Bb:261:ARG:HG3   | 9:Bb:323:TRP:CD2   | 2.55                     | 0.41              |
| 17:Bj:74:LEU:HD23  | 17:Bj:77:ILE:HD11  | 2.02                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 25:Bt:48:TRP:CH2   | 67:B3:121:PRO:HG3  | 2.55                     | 0.41              |
| 26:Bu:156:MET:HA   | 26:Bu:159:GLU:HG2  | 2.02                     | 0.41              |
| 28:B0:78:GLY:HA3   | 28:B0:132:HIS:CE1  | 2.55                     | 0.41              |
| 29:Bw:292:GLN:HG3  | 29:Bw:329:TRP:CZ3  | 2.55                     | 0.41              |
| 30:Bx:161:PRO:HA   | 82:BN:74:GLN:HA    | 2.01                     | 0.41              |
| 31:AA:55:G:C6      | 31:AA:63:G:N1      | 2.88                     | 0.41              |
| 31:AA:455:A:N7     | 31:AA:935:G:O2'    | 2.48                     | 0.41              |
| 34:AE:296:LEU:HG   | 34:AE:303:ILE:HB   | 2.02                     | 0.41              |
| 53:Ae:106:PRO:HB2  | 53:Ae:140:ASN:ND2  | 2.35                     | 0.41              |
| 56:Ag:122:ARG:HH11 | 56:Ag:336:LEU:HD13 | 1.84                     | 0.41              |
| 65:EL:74:LEU:HB3   | 65:EL:78:GLU:HB2   | 2.01                     | 0.41              |
| 31:BA:1331:G:O6    | 31:BA:1403:U:O4    | 2.37                     | 0.41              |
| 31:BA:1464:A:H4'   | 75:BC:55:ILE:HG21  | 2.00                     | 0.41              |
| 31:BA:1518:A:C2    | 31:BA:1528:A:C4    | 3.08                     | 0.41              |
| 1:AI:152:TYR:CZ    | 32:AB:189:PRO:HG3  | 2.55                     | 0.41              |
| 2:BT:96:ARG:O      | 2:BT:99:MET:HG2    | 2.20                     | 0.41              |
| 20:Bm:78:VAL:HG23  | 20:Bm:104:ARG:HH21 | 1.85                     | 0.41              |
| 20:Bm:157:TRP:CE2  | 20:Bm:159:TYR:HB2  | 2.55                     | 0.41              |
| 31:AA:198:C:H2'    | 31:AA:199:G:H8     | 1.84                     | 0.41              |
| 31:AA:589:C:H2'    | 31:AA:590:C:C6     | 2.54                     | 0.41              |
| 31:AA:591:A:H2'    | 31:AA:592:A:C8     | 2.55                     | 0.41              |
| 31:AA:619:C:H1'    | 37:AJ:124:VAL:HG23 | 2.00                     | 0.41              |
| 49:Aa:190:ARG:HH21 | 64:Ap:177:PHE:HD2  | 1.66                     | 0.41              |
| 54:B1:42:HIS:HE1   | 54:B1:83:GLU:HB2   | 1.84                     | 0.41              |
| 56:Ag:77:VAL:C     | 56:Ag:79:PRO:HD3   | 2.45                     | 0.41              |
| 62:An:151:ARG:NH2  | 31:BA:875:C:O2'    | 2.53                     | 0.41              |
| 63:Ao:611:ALA:HA   | 63:Ao:614:LEU:HD23 | 2.02                     | 0.41              |
| 65:EL:86:LEU:HD21  | 65:FL:71:ILE:HD11  | 2.01                     | 0.41              |
| 31:BA:306:A:H2'    | 31:BA:307:G:C8     | 2.55                     | 0.41              |
| 31:BA:840:C:H2'    | 31:BA:841:A:H8     | 1.85                     | 0.41              |
| 31:BA:1026:A:C6    | 31:BA:1321:C:H1'   | 2.55                     | 0.41              |
| 31:BA:1570:C:H3'   | 31:BA:1571:A:C8    | 2.54                     | 0.41              |
| 75:BC:54:HIS:O     | 75:BC:59:LYS:NZ    | 2.53                     | 0.41              |
| 76:BD:207:TYR:O    | 76:BD:209:ARG:HG3  | 2.20                     | 0.41              |
| 84:BP:260:LYS:NZ   | 84:BP:265:ILE:O    | 2.45                     | 0.41              |
| 86:BR:33:LEU:HD21  | 86:BR:59:LEU:HD22  | 2.02                     | 0.41              |
| 7:BY:133:VAL:HG13  | 7:BY:145:ARG:HB3   | 2.01                     | 0.41              |
| 9:Bb:195:PRO:HA    | 9:Bb:198:ALA:HB3   | 2.02                     | 0.41              |
| 31:AA:628:G:H2'    | 31:AA:629:C:C6     | 2.55                     | 0.41              |
| 36:AG:187:MET:HE1  | 36:AG:209:LEU:HD23 | 2.02                     | 0.41              |
| 38:AK:109:LEU:O    | 38:AK:144:LYS:NZ   | 2.36                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 38:AK:114:CYS:HB3  | 38:AK:124:LYS:HB2  | 2.02                     | 0.41              |
| 46:AV:41:A:H2'     | 46:AV:42:A:O4'     | 2.19                     | 0.41              |
| 59:Aj:82:ARG:HD3   | 59:Aj:85:TRP:CE2   | 2.55                     | 0.41              |
| 65:LL:134:LEU:HD23 | 65:LL:168:LEU:HD21 | 2.01                     | 0.41              |
| 31:BA:341:G:H2'    | 31:BA:342:C:C6     | 2.55                     | 0.41              |
| 31:BA:1125:U:H2'   | 31:BA:1126:U:C6    | 2.55                     | 0.41              |
| 31:BA:1329:U:OP2   | 31:BA:1399:G:N1    | 2.41                     | 0.41              |
| 75:BC:175:LYS:HB3  | 75:BC:178:ARG:HD3  | 2.02                     | 0.41              |
| 75:BC:553:ILE:HG13 | 75:BC:612:GLN:HB2  | 2.02                     | 0.41              |
| 82:BN:111:MET:HE2  | 82:BN:111:MET:HB3  | 1.91                     | 0.41              |
| 2:BT:140:ARG:HH21  | 2:BT:166:LEU:HD11  | 1.84                     | 0.41              |
| 9:Bb:237:VAL:HG22  | 9:Bb:240:ILE:HD11  | 2.03                     | 0.41              |
| 11:Bd:95:LEU:HD23  | 18:Bk:169:ILE:HD12 | 2.02                     | 0.41              |
| 15:Bh:216:ARG:HG3  | 15:Bh:220:ILE:HD12 | 2.02                     | 0.41              |
| 18:Bk:202:PRO:O    | 18:Bk:205:GLU:HG2  | 2.21                     | 0.41              |
| 31:AA:247:G:O2'    | 31:AA:262:C:O2'    | 2.36                     | 0.41              |
| 31:AA:438:C:H2'    | 31:AA:439:A:C8     | 2.55                     | 0.41              |
| 31:AA:727:C:H2'    | 31:AA:728:U:C6     | 2.54                     | 0.41              |
| 31:AA:810:C:H2'    | 31:AA:811:U:C6     | 2.54                     | 0.41              |
| 33:AC:92:LEU:HD13  | 33:AC:119:ILE:HD11 | 2.02                     | 0.41              |
| 36:AG:114:THR:HG21 | 36:AG:205:LEU:HD23 | 2.03                     | 0.41              |
| 43:AQ:14:VAL:H     | 51:Ac:63:GLN:HE22  | 1.68                     | 0.41              |
| 60:Ak:188:ALA:O    | 60:Ak:235:SER:OG   | 2.37                     | 0.41              |
| 72:B8:115:LEU:HB2  | 84:BP:83:PHE:HB3   | 2.02                     | 0.41              |
| 31:BA:645:U:H2'    | 31:BA:646:A:C8     | 2.55                     | 0.41              |
| 31:BA:657:U:H1'    | 31:BA:658:U:C5     | 2.55                     | 0.41              |
| 31:BA:1243:U:H2'   | 31:BA:1244:U:C6    | 2.55                     | 0.41              |
| 31:BA:1331:G:H1    | 31:BA:1403:U:H3    | 1.68                     | 0.41              |
| 75:BC:73:ILE:HD11  | 75:BC:88:VAL:HG11  | 2.03                     | 0.41              |
| 75:BC:262:GLU:OE1  | 75:BC:262:GLU:N    | 2.53                     | 0.41              |
| 77:BE:48:TRP:CE2   | 77:BE:51:GLU:HB2   | 2.55                     | 0.41              |
| 87:BS:65:GLU:HG3   | 87:BS:97:ARG:HD2   | 2.02                     | 0.41              |
| 1:AI:143:ASP:OD1   | 1:AI:143:ASP:N     | 2.52                     | 0.41              |
| 2:BT:191:ARG:HE    | 83:BO:99:ARG:HH22  | 1.68                     | 0.41              |
| 8:Ba:113:LEU:HD23  | 8:Ba:119:GLN:HB2   | 2.01                     | 0.41              |
| 9:Bb:106:ARG:NH1   | 74:BB:23:A:OP2     | 2.44                     | 0.41              |
| 9:Bb:358:PRO:HG2   | 72:B8:149:PHE:HD2  | 1.86                     | 0.41              |
| 16:Bi:173:VAL:HA   | 16:Bi:176:ILE:HG22 | 2.01                     | 0.41              |
| 17:Bj:235:LYS:HE3  | 17:Bj:275:PHE:CD1  | 2.56                     | 0.41              |
| 19:Bl:98:ARG:HH21  | 19:Bl:154:ASP:CG   | 2.29                     | 0.41              |
| 31:AA:13:U:H2'     | 31:AA:14:C:H6      | 1.85                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:AA:26:A:H2'     | 31:AA:27:U:C6      | 2.56                     | 0.41              |
| 31:AA:199:G:N2     | 31:AA:201:A:H3'    | 2.35                     | 0.41              |
| 31:AA:408:A:H4'    | 31:AA:949:G:N2     | 2.35                     | 0.41              |
| 31:AA:532:G:H2'    | 31:AA:533:C:C6     | 2.55                     | 0.41              |
| 31:AA:583:A:C8     | 31:AA:584:C:H5     | 2.39                     | 0.41              |
| 31:AA:650:A:H61    | 32:AB:176:THR:HG21 | 1.86                     | 0.41              |
| 32:AB:252:PHE:O    | 32:AB:256:ILE:HG12 | 2.19                     | 0.41              |
| 53:Ae:433:ARG:O    | 53:Ae:436:GLU:HG3  | 2.21                     | 0.41              |
| 56:Ag:264:VAL:HG22 | 56:Ag:268:TRP:HZ3  | 1.84                     | 0.41              |
| 60:Ak:105:LEU:HG   | 60:Ak:109:LYS:HE3  | 2.02                     | 0.41              |
| 63:Ao:267:ARG:HH22 | 63:Ao:295:TYR:HB3  | 1.85                     | 0.41              |
| 65:DL:75:THR:HG22  | 65:DL:78:GLU:HG3   | 2.01                     | 0.41              |
| 65:FL:70:ASP:OD1   | 65:FL:71:ILE:N     | 2.53                     | 0.41              |
| 31:BA:1031:C:H2'   | 31:BA:1032:G:C8    | 2.55                     | 0.41              |
| 31:BA:1492:C:C4    | 86:BR:15:PHE:HB2   | 2.56                     | 0.41              |
| 77:BE:96:ARG:NH2   | 77:BE:301:ASP:OD1  | 2.54                     | 0.41              |
| 78:BF:182:LEU:HD13 | 78:BF:187:LEU:HD23 | 2.02                     | 0.41              |
| 81:BK:157:LYS:HG3  | 81:BK:158:ASP:H    | 1.85                     | 0.41              |
| 82:BN:38:LYS:HG3   | 82:BN:145:LEU:HD11 | 2.02                     | 0.41              |
| 83:BO:43:ASN:HD21  | 83:BO:118:ARG:HG2  | 1.84                     | 0.41              |
| 86:BR:28:LEU:HD13  | 86:BR:48:ARG:HH12  | 1.86                     | 0.41              |
| 1:AI:88:LEU:HA     | 1:AI:91:MET:HG2    | 2.02                     | 0.41              |
| 8:Ba:260:SER:OG    | 76:BD:147:ASN:OD1  | 2.22                     | 0.41              |
| 15:Bh:81:GLU:OE1   | 15:Bh:210:ARG:NE   | 2.53                     | 0.41              |
| 31:AA:28:U:H2'     | 31:AA:29:A:H8      | 1.86                     | 0.41              |
| 31:AA:501:C:H2'    | 31:AA:503:A:C8     | 2.56                     | 0.41              |
| 31:AA:512:A:H2'    | 31:AA:513:A:C8     | 2.56                     | 0.41              |
| 31:AA:821:A:OP1    | 36:AG:177:ARG:NH1  | 2.53                     | 0.41              |
| 34:AE:259:GLY:HA3  | 34:AE:271:ALA:HB2  | 2.03                     | 0.41              |
| 50:Ab:28:LYS:HE3   | 50:Ab:32:LEU:HD23  | 2.03                     | 0.41              |
| 69:B5:139:ARG:NH2  | 31:BA:656:C:OP2    | 2.51                     | 0.41              |
| 70:B6:31:ASN:HB2   | 72:B8:134:TRP:HB3  | 2.01                     | 0.41              |
| 31:BA:5:A:C6       | 31:BA:6:A:C6       | 3.08                     | 0.41              |
| 31:BA:211:U:H2'    | 31:BA:212:C:H6     | 1.85                     | 0.41              |
| 31:BA:234:G:H2'    | 31:BA:235:A:C8     | 2.56                     | 0.41              |
| 31:BA:266:C:H5''   | 31:BA:267:A:H5'    | 2.02                     | 0.41              |
| 31:BA:302:A:H2'    | 31:BA:303:G:C8     | 2.56                     | 0.41              |
| 31:BA:787:U:H2'    | 31:BA:788:A:O4'    | 2.20                     | 0.41              |
| 31:BA:1089:G:OP1   | 79:BI:121:ASN:ND2  | 2.53                     | 0.41              |
| 31:BA:1147:G:N1    | 31:BA:1158:C:N3    | 2.69                     | 0.41              |
| 31:BA:1215:C:H42   | 31:BA:1220:A:N6    | 2.19                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:BA:1222:A:H2'   | 31:BA:1223:U:H6    | 1.85                     | 0.41              |
| 31:BA:1430:G:H2'   | 31:BA:1431:G:C8    | 2.56                     | 0.41              |
| 81:BK:103:HIS:O    | 81:BK:107:GLU:HG2  | 2.20                     | 0.41              |
| 87:BS:54:ARG:HG3   | 87:BS:58:LEU:HG    | 2.02                     | 0.41              |
| 15:Bh:287:GLU:OE1  | 15:Bh:287:GLU:N    | 2.43                     | 0.41              |
| 16:Bi:124:LYS:O    | 16:Bi:127:GLU:HG3  | 2.21                     | 0.41              |
| 31:AA:58:U:N3      | 59:Aj:57:ASP:OD2   | 2.53                     | 0.41              |
| 31:AA:756:U:H2'    | 31:AA:757:U:C6     | 2.56                     | 0.41              |
| 33:AC:99:THR:O     | 33:AC:101:PRO:HD3  | 2.20                     | 0.41              |
| 34:AE:283:GLU:O    | 34:AE:356:GLN:NE2  | 2.36                     | 0.41              |
| 36:AG:52:ARG:HA    | 36:AG:52:ARG:HD3   | 1.89                     | 0.41              |
| 37:AJ:122:LYS:O    | 40:AN:112:ARG:NH1  | 2.49                     | 0.41              |
| 40:AN:81:ASP:HA    | 40:AN:86:ARG:HD3   | 2.02                     | 0.41              |
| 43:AQ:86:PHE:HZ    | 51:Ac:75:PHE:HZ    | 1.69                     | 0.41              |
| 45:AU:67:GLU:HG3   | 55:Af:155:LEU:HG   | 2.01                     | 0.41              |
| 53:Ae:166:LEU:HD11 | 53:Ae:202:SER:HB2  | 2.03                     | 0.41              |
| 55:Af:81:PHE:CZ    | 55:Af:85:LEU:HD22  | 2.55                     | 0.41              |
| 55:Af:149:GLU:HG2  | 55:Af:151:THR:HG23 | 2.03                     | 0.41              |
| 31:BA:225:C:H2'    | 31:BA:226:U:C6     | 2.55                     | 0.41              |
| 31:BA:682:G:H2'    | 31:BA:683:U:C6     | 2.56                     | 0.41              |
| 31:BA:693:U:O2'    | 31:BA:694:A:H5'    | 2.20                     | 0.41              |
| 31:BA:1343:C:H2'   | 31:BA:1344:C:C6    | 2.56                     | 0.41              |
| 78:BF:83:HIS:CD2   | 78:BF:85:ASP:HB2   | 2.55                     | 0.41              |
| 84:BP:156:VAL:O    | 84:BP:176:THR:HA   | 2.21                     | 0.41              |
| 85:BQ:105:MET:SD   | 85:BQ:183:LEU:HD21 | 2.61                     | 0.41              |
| 3:BU:31:PHE:CE1    | 31:BA:165:A:H5''   | 2.56                     | 0.41              |
| 5:BW:90:LYS:HD2    | 5:BW:93:ARG:HD2    | 2.02                     | 0.41              |
| 8:Ba:64:MET:HA     | 66:B2:190:TRP:CE2  | 2.56                     | 0.41              |
| 11:Bd:136:PRO:HB3  | 17:Bj:153:LEU:HD13 | 2.02                     | 0.41              |
| 12:Be:32:LYS:HE2   | 12:Be:32:LYS:HB3   | 1.88                     | 0.41              |
| 17:Bj:170:ILE:HG13 | 17:Bj:172:MET:HB2  | 2.03                     | 0.41              |
| 22:Bo:23:ALA:N     | 31:BA:482:G:OP1    | 2.53                     | 0.41              |
| 27:Bv:129:PRO:HA   | 27:Bv:132:ILE:HG12 | 2.03                     | 0.41              |
| 31:AA:217:U:H2'    | 31:AA:218:A:C8     | 2.55                     | 0.41              |
| 31:AA:394:U:O2'    | 41:AO:129:ARG:NH1  | 2.53                     | 0.41              |
| 31:AA:581:A:OP2    | 31:AA:802:A:O2'    | 2.38                     | 0.41              |
| 31:AA:791:G:O2'    | 31:AA:817:G:O6     | 2.38                     | 0.41              |
| 31:AA:921:U:O2'    | 31:BA:914:A:N1     | 2.44                     | 0.41              |
| 31:AA:940:C:H2'    | 31:AA:941:U:H6     | 1.85                     | 0.41              |
| 32:AB:269:LEU:O    | 32:AB:273:GLN:HG3  | 2.21                     | 0.41              |
| 37:AJ:72:LEU:HB3   | 37:AJ:177:LEU:HD12 | 2.02                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 37:AJ:76:LEU:HD23  | 37:AJ:145:LEU:HD12 | 2.03                     | 0.41              |
| 53:Ae:112:ILE:HG23 | 53:Ae:148:THR:HG21 | 2.03                     | 0.41              |
| 54:B1:189:ASP:HA   | 54:B1:192:LYS:HG2  | 2.01                     | 0.41              |
| 56:Ag:144:CYS:SG   | 56:Ag:258:LEU:HD22 | 2.60                     | 0.41              |
| 63:Ao:282:TYR:O    | 63:Ao:285:LEU:HG   | 2.20                     | 0.41              |
| 63:Ao:559:LYS:HE3  | 63:Ao:574:TRP:HZ2  | 1.85                     | 0.41              |
| 67:B3:64:HIS:O     | 67:B3:102:ASN:ND2  | 2.50                     | 0.41              |
| 31:BA:184:U:OP1    | 84:BP:53:HIS:NE2   | 2.54                     | 0.41              |
| 31:BA:906:G:H2'    | 31:BA:907:U:O4'    | 2.21                     | 0.41              |
| 31:BA:1191:A:H2'   | 31:BA:1192:U:H6    | 1.86                     | 0.41              |
| 31:BA:1308:A:P     | 85:BQ:101:HIS:HE2  | 2.44                     | 0.41              |
| 75:BC:528:THR:OG1  | 75:BC:529:ILE:N    | 2.53                     | 0.41              |
| 80:BJ:41:HIS:HD2   | 80:BJ:43:GLU:H     | 1.68                     | 0.41              |
| 80:BJ:121:ILE:HD13 | 80:BJ:164:MET:HE3  | 2.02                     | 0.41              |
| 1:AI:263:TYR:HD2   | 1:AI:268:MET:HA    | 1.85                     | 0.41              |
| 4:BV:181:ARG:NH1   | 31:BA:189:A:OP2    | 2.54                     | 0.41              |
| 8:Ba:113:LEU:HD22  | 8:Ba:311:ALA:HB1   | 2.03                     | 0.41              |
| 9:Bb:93:PRO:HD3    | 22:Bo:117:LEU:HB2  | 2.03                     | 0.41              |
| 9:Bb:152:ALA:HA    | 9:Bb:157:LEU:HD23  | 2.02                     | 0.41              |
| 10:Bc:181:VAL:HG22 | 10:Bc:290:VAL:HG22 | 2.02                     | 0.41              |
| 12:Be:51:ILE:HA    | 31:BA:747:U:H3     | 1.85                     | 0.41              |
| 16:Bi:140:LYS:HZ1  | 16:Bi:259:TRP:CD1  | 2.39                     | 0.41              |
| 16:Bi:176:ILE:HD12 | 16:Bi:176:ILE:HA   | 1.91                     | 0.41              |
| 18:Bk:137:LEU:HD21 | 18:Bk:141:GLY:HA2  | 2.02                     | 0.41              |
| 19:Bl:113:VAL:HG11 | 19:Bl:117:ILE:HG23 | 2.02                     | 0.41              |
| 22:Bo:84:MET:HE1   | 67:B3:101:LYS:HB3  | 2.03                     | 0.41              |
| 23:Bp:19:GLN:HA    | 23:Bp:54:ASP:HB3   | 2.03                     | 0.41              |
| 24:Bq:64:ASP:HA    | 24:Bq:68:LEU:HG    | 2.02                     | 0.41              |
| 31:AA:576:C:P      | 31:AA:715:G:H21    | 2.44                     | 0.41              |
| 31:AA:618:G:H21    | 31:AA:687:A:H62    | 1.69                     | 0.41              |
| 31:AA:738:U:H2'    | 36:AG:198:ARG:HE   | 1.85                     | 0.41              |
| 31:AA:759:U:H2'    | 31:AA:760:A:C8     | 2.55                     | 0.41              |
| 31:AA:771:A:H2'    | 31:AA:772:A:C8     | 2.55                     | 0.41              |
| 31:AA:787:A:H2'    | 31:AA:788:G:C8     | 2.56                     | 0.41              |
| 31:AA:945:A:OP1    | 62:An:141:HIS:NE2  | 2.48                     | 0.41              |
| 32:AB:56:ASP:OD1   | 32:AB:56:ASP:N     | 2.54                     | 0.41              |
| 34:AE:142:PRO:HA   | 34:AE:146:ILE:HG13 | 2.03                     | 0.41              |
| 36:AG:172:VAL:HG22 | 36:AG:240:ARG:HD3  | 2.02                     | 0.41              |
| 37:AJ:180:LEU:HD23 | 60:Ak:151:ILE:HD11 | 2.02                     | 0.41              |
| 40:AN:53:ARG:HH21  | 57:Ah:364:HIS:CD2  | 2.39                     | 0.41              |
| 41:AO:127:GLU:CD   | 41:AO:127:GLU:H    | 2.25                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 42:AP:95:GLY:O     | 59:Aj:167:PRO:HB2  | 2.21                     | 0.41              |
| 49:Aa:158:ALA:O    | 49:Aa:208:TRP:NE1  | 2.42                     | 0.41              |
| 53:Ae:106:PRO:HB3  | 53:Ae:139:PRO:HD2  | 2.02                     | 0.41              |
| 53:Ae:243:ASN:OD1  | 53:Ae:244:PHE:N    | 2.54                     | 0.41              |
| 60:Ak:268:LEU:HB3  | 60:Ak:285:LEU:HD22 | 2.02                     | 0.41              |
| 61:Am:57:LYS:HD2   | 61:Am:57:LYS:HA    | 1.88                     | 0.41              |
| 63:Ao:116:ALA:O    | 63:Ao:120:ILE:HG12 | 2.20                     | 0.41              |
| 63:Ao:129:GLN:NE2  | 63:Ao:144:TYR:OH   | 2.39                     | 0.41              |
| 63:Ao:469:CYS:SG   | 63:Ao:498:ASP:HB3  | 2.61                     | 0.41              |
| 65:EL:85:LEU:HA    | 65:EL:88:LYS:HG2   | 2.01                     | 0.41              |
| 70:B6:17:LEU:HD11  | 70:B6:31:ASN:HB3   | 2.02                     | 0.41              |
| 31:BA:208:A:H2'    | 31:BA:209:A:H8     | 1.86                     | 0.41              |
| 31:BA:209:A:H2     | 31:BA:426:A:H4'    | 1.86                     | 0.41              |
| 31:BA:347:U:O4'    | 31:BA:349:A:H5'    | 2.21                     | 0.41              |
| 31:BA:348:G:C8     | 78:BF:118:ALA:HB2  | 2.56                     | 0.41              |
| 31:BA:838:A:H1'    | 31:BA:933:A:H61    | 1.85                     | 0.41              |
| 31:BA:974:C:H2'    | 31:BA:975:G:H8     | 1.85                     | 0.41              |
| 31:BA:981:U:H2'    | 31:BA:982:U:C6     | 2.56                     | 0.41              |
| 31:BA:1019:C:H2'   | 31:BA:1020:C:C6    | 2.56                     | 0.41              |
| 31:BA:1040:A:C2    | 31:BA:1041:A:C8    | 3.08                     | 0.41              |
| 74:BB:65:U:H2'     | 74:BB:66:A:C8      | 2.55                     | 0.41              |
| 75:BC:138:LEU:HD23 | 75:BC:417:ILE:HD11 | 2.03                     | 0.41              |
| 75:BC:324:GLN:HB3  | 75:BC:342:LEU:HD11 | 2.03                     | 0.41              |
| 75:BC:571:ASP:OD1  | 75:BC:571:ASP:N    | 2.54                     | 0.41              |
| 94:BC:802:GNP:O2A  | 95:BC:901:HOH:O    | 2.21                     | 0.41              |
| 76:BD:199:SER:HB2  | 76:BD:203:ARG:HD3  | 2.03                     | 0.41              |
| 76:BD:222:ASN:O    | 76:BD:222:ASN:ND2  | 2.54                     | 0.41              |
| 77:BE:109:LEU:HD21 | 77:BE:337:VAL:HG22 | 2.03                     | 0.41              |
| 77:BE:149:GLY:O    | 77:BE:173:LYS:HD2  | 2.21                     | 0.41              |
| 78:BF:222:GLU:HB2  | 78:BF:225:ASP:HB2  | 2.03                     | 0.41              |
| 79:BI:59:TRP:NE1   | 79:BI:81:LYS:HB3   | 2.36                     | 0.41              |
| 83:BO:72:ARG:HD3   | 83:BO:83:LYS:HD3   | 2.01                     | 0.41              |
| 84:BP:111:ASP:OD1  | 84:BP:111:ASP:N    | 2.51                     | 0.41              |
| 1:AI:295:ASP:HB3   | 1:AI:330:THR:HG22  | 2.02                     | 0.41              |
| 5:BW:75:ARG:HB3    | 5:BW:78:ILE:HD11   | 2.03                     | 0.41              |
| 7:BY:52:GLU:HB3    | 7:BY:143:ARG:HH22  | 1.85                     | 0.41              |
| 16:Bi:292:GLU:OE2  | 69:B5:179:ARG:NH2  | 2.54                     | 0.41              |
| 29:Bw:203:PHE:HE1  | 29:Bw:224:ARG:HB3  | 1.86                     | 0.41              |
| 29:Bw:241:LEU:HD11 | 29:Bw:290:HIS:HD1  | 1.85                     | 0.41              |
| 30:Bx:75:TRP:CD1   | 82:BN:169:VAL:HG13 | 2.56                     | 0.41              |
| 31:AA:229:U:H2'    | 31:AA:230:U:C6     | 2.56                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 31:AA:238:C:H2'    | 31:AA:239:U:H6     | 1.86                     | 0.41              |
| 31:AA:816:U:H2'    | 31:AA:817:G:O4'    | 2.20                     | 0.41              |
| 31:AA:829:G:H2'    | 31:AA:830:A:H8     | 1.86                     | 0.41              |
| 31:AA:866:U:H2'    | 31:AA:867:G:C8     | 2.55                     | 0.41              |
| 33:AC:108:LEU:HD23 | 33:AC:110:LEU:HD21 | 2.02                     | 0.41              |
| 36:AG:139:ARG:HH22 | 56:Ag:363:ASN:HD22 | 1.69                     | 0.41              |
| 42:AP:29:ARG:HG2   | 51:Ac:141:CYS:SG   | 2.61                     | 0.41              |
| 49:Aa:298:VAL:HA   | 49:Aa:303:ILE:HD11 | 2.03                     | 0.41              |
| 55:Af:115:ILE:HD13 | 55:Af:141:VAL:HG21 | 2.02                     | 0.41              |
| 56:Ag:323:LEU:HB2  | 56:Ag:326:GLU:HG2  | 2.03                     | 0.41              |
| 60:Ak:177:VAL:HG13 | 60:Ak:207:LEU:HB3  | 2.02                     | 0.41              |
| 31:BA:410:U:C4     | 31:BA:411:U:O4     | 2.74                     | 0.41              |
| 31:BA:498:A:H3'    | 31:BA:499:C:C6     | 2.56                     | 0.41              |
| 31:BA:864:U:H2'    | 31:BA:865:A:H8     | 1.84                     | 0.41              |
| 31:BA:920:C:O2     | 31:BA:924:G:O6     | 2.38                     | 0.41              |
| 77:BE:205:ASP:CG   | 77:BE:302:SER:HA   | 2.46                     | 0.41              |
| 78:BF:108:ARG:HD3  | 78:BF:161:TYR:CD1  | 2.55                     | 0.41              |
| 80:BJ:107:GLU:H    | 80:BJ:107:GLU:CD   | 2.29                     | 0.41              |
| 8:Ba:188:CYS:HB3   | 8:Ba:418:TYR:CD2   | 2.56                     | 0.40              |
| 8:Ba:355:LEU:HD13  | 8:Ba:376:VAL:HG22  | 2.03                     | 0.40              |
| 10:Bc:190:MET:HG2  | 10:Bc:291:ARG:NH1  | 2.36                     | 0.40              |
| 16:Bi:160:LEU:O    | 16:Bi:164:VAL:HG22 | 2.21                     | 0.40              |
| 27:Bv:131:MET:HE1  | 70:B6:23:GLN:HB3   | 2.03                     | 0.40              |
| 29:Bw:267:LEU:HD23 | 29:Bw:267:LEU:HA   | 1.91                     | 0.40              |
| 31:AA:70:U:H2'     | 31:AA:71:G:H8      | 1.85                     | 0.40              |
| 31:AA:265:U:H2'    | 31:AA:266:U:C6     | 2.56                     | 0.40              |
| 31:AA:493:A:N1     | 31:AA:511:A:H5''   | 2.36                     | 0.40              |
| 34:AE:294:ILE:HG23 | 34:AE:305:MET:HB2  | 2.01                     | 0.40              |
| 36:AG:57:GLU:HG3   | 36:AG:60:GLU:HB3   | 2.03                     | 0.40              |
| 42:AP:30:PRO:HG2   | 42:AP:56:PRO:HG2   | 2.02                     | 0.40              |
| 42:AP:90:LEU:HD13  | 42:AP:90:LEU:HA    | 1.98                     | 0.40              |
| 42:AP:100:HIS:CD2  | 42:AP:102:MET:HB2  | 2.56                     | 0.40              |
| 49:Aa:224:ARG:HH21 | 64:Ap:173:ARG:HB2  | 1.85                     | 0.40              |
| 53:Ae:406:PRO:HA   | 53:Ae:409:GLU:HG2  | 2.02                     | 0.40              |
| 57:Ah:296:TRP:CD1  | 57:Ah:301:LYS:HD2  | 2.56                     | 0.40              |
| 31:BA:484:A:C2     | 31:BA:584:A:C4     | 3.09                     | 0.40              |
| 31:BA:516:G:H8     | 31:BA:516:G:P      | 2.44                     | 0.40              |
| 75:BC:563:ASP:O    | 75:BC:565:THR:OG1  | 2.35                     | 0.40              |
| 78:BF:284:TYR:HB2  | 78:BF:288:LEU:HD12 | 2.03                     | 0.40              |
| 9:Bb:139:TRP:O     | 9:Bb:144:GLY:N     | 2.47                     | 0.40              |
| 11:Bd:105:GLU:CD   | 17:Bj:212:HIS:HB3  | 2.46                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:Bq:77:ILE:HG12  | 81:BK:85:PRO:HG2   | 2.03                     | 0.40              |
| 29:Bw:105:TRP:CD1  | 29:Bw:265:LEU:HD13 | 2.56                     | 0.40              |
| 31:AA:81:U:O4      | 31:AA:102:G:N1     | 2.55                     | 0.40              |
| 31:AA:355:U:H2'    | 31:AA:356:A:C8     | 2.51                     | 0.40              |
| 31:AA:387:C:H2'    | 31:AA:388:U:H6     | 1.87                     | 0.40              |
| 31:AA:388:U:C2     | 31:AA:389:A:C8     | 3.08                     | 0.40              |
| 34:AE:418:LYS:HD3  | 34:AE:418:LYS:HA   | 1.97                     | 0.40              |
| 34:AE:426:LYS:HB3  | 64:Ap:136:HIS:CD2  | 2.57                     | 0.40              |
| 36:AG:161:ILE:HD12 | 36:AG:170:VAL:HG21 | 2.03                     | 0.40              |
| 54:B1:132:LEU:HB3  | 79:BI:120:ARG:NE   | 2.36                     | 0.40              |
| 57:Ah:367:TRP:HA   | 57:Ah:370:ASN:ND2  | 2.35                     | 0.40              |
| 67:B3:51:GLU:OE1   | 67:B3:51:GLU:N     | 2.54                     | 0.40              |
| 31:BA:64:C:H2'     | 31:BA:65:C:O4'     | 2.21                     | 0.40              |
| 31:BA:190:U:O4     | 31:BA:1024:G:O2'   | 2.22                     | 0.40              |
| 31:BA:562:A:N6     | 31:BA:1287:G:H1'   | 2.36                     | 0.40              |
| 31:BA:1013:A:H2'   | 31:BA:1014:A:C8    | 2.55                     | 0.40              |
| 31:BA:1425:A:OP1   | 31:BA:1425:A:H3'   | 2.21                     | 0.40              |
| 75:BC:125:VAL:HG22 | 75:BC:154:GLN:HE21 | 1.86                     | 0.40              |
| 75:BC:671:ARG:NH2  | 75:BC:702:GLU:OE1  | 2.50                     | 0.40              |
| 76:BD:85:ARG:NE    | 76:BD:91:ILE:HG12  | 2.37                     | 0.40              |
| 78:BF:69:LEU:HB2   | 78:BF:190:VAL:HG11 | 2.03                     | 0.40              |
| 83:BO:88:GLY:HA3   | 83:BO:100:PHE:CD1  | 2.56                     | 0.40              |
| 84:BP:38:ARG:HD3   | 84:BP:45:ARG:HH21  | 1.86                     | 0.40              |
| 6:BX:140:ARG:HG3   | 10:Bc:77:VAL:HG21  | 2.02                     | 0.40              |
| 7:BY:72:LYS:HB3    | 16:Bi:256:TYR:OH   | 2.20                     | 0.40              |
| 10:Bc:212:PRO:HG3  | 10:Bc:268:ARG:NH1  | 2.37                     | 0.40              |
| 10:Bc:298:LEU:HG   | 10:Bc:309:TRP:HZ3  | 1.86                     | 0.40              |
| 13:Bf:109:ILE:HG23 | 13:Bf:123:TRP:HB2  | 2.04                     | 0.40              |
| 17:Bj:71:ALA:HB2   | 68:B4:41:LEU:HD22  | 2.02                     | 0.40              |
| 17:Bj:243:PHE:HZ   | 17:Bj:248:LYS:HE2  | 1.86                     | 0.40              |
| 20:Bm:57:GLN:O     | 78:BF:211:ARG:NH2  | 2.55                     | 0.40              |
| 30:Bx:117:GLU:HG3  | 30:Bx:180:LEU:HD12 | 2.04                     | 0.40              |
| 31:AA:388:U:H4'    | 35:AF:72:ALA:HB1   | 2.03                     | 0.40              |
| 32:AB:105:LEU:HD21 | 32:AB:224:THR:HG22 | 2.03                     | 0.40              |
| 32:AB:218:THR:HG22 | 32:AB:231:ILE:HG23 | 2.02                     | 0.40              |
| 49:Aa:151:PRO:HA   | 49:Aa:152:PRO:HD3  | 1.94                     | 0.40              |
| 52:Ad:134:ARG:HA   | 52:Ad:137:GLU:HG2  | 2.03                     | 0.40              |
| 53:Ae:168:THR:HA   | 53:Ae:171:ASN:HD21 | 1.86                     | 0.40              |
| 56:Ag:105:LEU:HD23 | 56:Ag:108:LEU:HD21 | 2.03                     | 0.40              |
| 56:Ag:323:LEU:HB3  | 60:Ak:306:ASP:OD2  | 2.22                     | 0.40              |
| 56:Ag:348:ASN:H    | 56:Ag:351:GLU:HB2  | 1.86                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 65:LL:133:ARG:HG2  | 65:LL:171:GLU:HA   | 2.04                     | 0.40              |
| 72:B8:140:ARG:N    | 72:B8:143:ARG:HH21 | 2.19                     | 0.40              |
| 31:BA:57:A:H4'     | 31:BA:1064:G:OP2   | 2.21                     | 0.40              |
| 31:BA:619:C:N4     | 31:BA:620:A:H62    | 2.20                     | 0.40              |
| 31:BA:672:G:H2'    | 31:BA:673:C:C6     | 2.56                     | 0.40              |
| 31:BA:811:A:N3     | 77:BE:230:THR:HG21 | 2.35                     | 0.40              |
| 31:BA:824:G:N2     | 31:BA:826:C:H5''   | 2.36                     | 0.40              |
| 77:BE:218:VAL:HG11 | 77:BE:240:PRO:HB3  | 2.04                     | 0.40              |
| 78:BF:187:LEU:HD13 | 78:BF:259:LEU:HD23 | 2.03                     | 0.40              |
| 3:BU:98:ASN:H      | 4:BV:109:GLN:NE2   | 2.19                     | 0.40              |
| 10:Bc:127:PHE:HB3  | 10:Bc:302:LEU:HD11 | 2.03                     | 0.40              |
| 11:Bd:23:ARG:NH1   | 46:AV:43:A:H4'     | 2.37                     | 0.40              |
| 13:Bf:128:GLN:O    | 13:Bf:132:ARG:HG2  | 2.21                     | 0.40              |
| 15:Bh:245:LEU:HB3  | 15:Bh:250:ILE:HB   | 2.03                     | 0.40              |
| 20:Bm:118:LEU:HD11 | 78:BF:65:TRP:CD1   | 2.56                     | 0.40              |
| 29:Bw:326:LEU:HD21 | 29:Bw:353:GLY:HA3  | 2.03                     | 0.40              |
| 31:AA:79:C:H2'     | 31:AA:80:C:H6      | 1.86                     | 0.40              |
| 31:AA:246:A:OP1    | 39:AL:77:ASN:HB2   | 2.21                     | 0.40              |
| 31:AA:268:A:H2'    | 31:AA:269:C:C6     | 2.56                     | 0.40              |
| 31:AA:446:C:C2     | 31:AA:447:U:C5     | 3.10                     | 0.40              |
| 34:AE:244:LEU:HD12 | 34:AE:257:ALA:O    | 2.22                     | 0.40              |
| 38:AK:102:VAL:HA   | 38:AK:108:PRO:HA   | 2.03                     | 0.40              |
| 39:AL:103:GLN:HG2  | 75:BC:484:PHE:HB3  | 2.02                     | 0.40              |
| 40:AN:36:ARG:O     | 40:AN:40:ARG:HG3   | 2.21                     | 0.40              |
| 41:AO:99:ALA:HB1   | 41:AO:103:GLU:HG3  | 2.04                     | 0.40              |
| 50:Ab:48:ARG:HA    | 50:Ab:49:PRO:HD3   | 1.89                     | 0.40              |
| 54:B1:100:ARG:NH2  | 31:BA:61:U:OP2     | 2.53                     | 0.40              |
| 56:Ag:69:ILE:HB    | 56:Ag:96:ALA:HB3   | 2.04                     | 0.40              |
| 63:Ao:526:PHE:O    | 63:Ao:530:LEU:HB2  | 2.20                     | 0.40              |
| 63:Ao:563:GLU:H    | 63:Ao:563:GLU:HG3  | 1.72                     | 0.40              |
| 65:DL:74:LEU:HB3   | 65:DL:78:GLU:HB2   | 2.03                     | 0.40              |
| 67:B3:73:LYS:HA    | 31:BA:472:U:OP1    | 2.21                     | 0.40              |
| 69:B5:125:TYR:O    | 69:B5:129:LYS:HG3  | 2.21                     | 0.40              |
| 31:BA:493:A:OP2    | 31:BA:1527:U:N3    | 2.42                     | 0.40              |
| 31:BA:677:C:OP1    | 31:BA:695:U:O2'    | 2.30                     | 0.40              |
| 31:BA:1269:G:N2    | 31:BA:1272:U:O2    | 2.42                     | 0.40              |
| 78:BF:114:THR:O    | 78:BF:156:ARG:NH1  | 2.54                     | 0.40              |
| 3:BU:101:VAL:HG11  | 4:BV:102:VAL:HG11  | 2.04                     | 0.40              |
| 6:BX:139:PRO:O     | 16:Bi:280:VAL:HG11 | 2.21                     | 0.40              |
| 7:BY:190:ARG:NE    | 7:BY:197:GLU:OE2   | 2.54                     | 0.40              |
| 8:Ba:96:HIS:CG     | 8:Ba:97:PRO:HD2    | 2.56                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 16:Bi:189:LEU:HB2  | 16:Bi:217:HIS:HD2  | 1.86                     | 0.40              |
| 20:Bm:115:ASN:OD1  | 20:Bm:115:ASN:N    | 2.55                     | 0.40              |
| 23:Bp:93:HIS:CE1   | 30:Bx:47:THR:HG21  | 2.56                     | 0.40              |
| 29:Bw:201:HIS:CD2  | 29:Bw:228:ASN:HD22 | 2.38                     | 0.40              |
| 31:AA:450:C:OP1    | 31:AA:502:A:N6     | 2.48                     | 0.40              |
| 31:AA:751:A:H1'    | 31:AA:753:A:N7     | 2.36                     | 0.40              |
| 32:AB:178:ALA:HB3  | 32:AB:179:PRO:HD3  | 2.03                     | 0.40              |
| 33:AC:131:LYS:HE3  | 34:AE:144:LEU:HD22 | 2.04                     | 0.40              |
| 34:AE:141:TRP:H    | 34:AE:145:ASN:HD22 | 1.68                     | 0.40              |
| 35:AF:8:LEU:HD11   | 35:AF:88:VAL:HG22  | 2.02                     | 0.40              |
| 53:Ae:249:LEU:HD13 | 53:Ae:249:LEU:HA   | 1.92                     | 0.40              |
| 54:B1:78:GLY:HA3   | 54:B1:126:THR:HG23 | 2.03                     | 0.40              |
| 61:Am:87:ARG:HA    | 61:Am:87:ARG:HD3   | 1.90                     | 0.40              |
| 63:Ao:608:ILE:HG21 | 63:Ao:642:LEU:HD21 | 2.03                     | 0.40              |
| 65:CL:64:ILE:HG23  | 65:DL:82:LEU:HD13  | 2.03                     | 0.40              |
| 67:B3:38:ARG:NH1   | 31:BA:410:U:OP1    | 2.43                     | 0.40              |
| 70:B6:20:MET:HB2   | 70:B6:30:PHE:CE2   | 2.57                     | 0.40              |
| 31:BA:64:C:H5''    | 79:BI:72:ARG:HH21  | 1.87                     | 0.40              |
| 31:BA:74:A:OP2     | 31:BA:75:A:O2'     | 2.36                     | 0.40              |
| 31:BA:189:A:H61    | 31:BA:1024:G:H21   | 1.70                     | 0.40              |
| 31:BA:365:G:N1     | 31:BA:598:U:OP2    | 2.54                     | 0.40              |
| 31:BA:407:A:H62    | 31:BA:1167:C:H2'   | 1.86                     | 0.40              |
| 31:BA:523:U:O2'    | 31:BA:532:A:OP1    | 2.39                     | 0.40              |
| 31:BA:783:A:O2'    | 31:BA:785:A:OP2    | 2.27                     | 0.40              |
| 75:BC:54:HIS:O     | 75:BC:57:SER:OG    | 2.31                     | 0.40              |
| 80:BJ:40:MET:HE2   | 85:BQ:242:TRP:CG   | 2.56                     | 0.40              |
| 81:BK:156:VAL:HG21 | 81:BK:159:LEU:HD12 | 2.03                     | 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   | AI    | 326/397 (82%) | 318 (98%)  | 8 (2%)  | 0        | 100         | 100 |
| 2   | BT    | 220/292 (75%) | 217 (99%)  | 3 (1%)  | 0        | 100         | 100 |
| 3   | BU    | 138/149 (93%) | 137 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 4   | BV    | 153/209 (73%) | 149 (97%)  | 4 (3%)  | 0        | 100         | 100 |
| 5   | BW    | 164/210 (78%) | 158 (96%)  | 6 (4%)  | 0        | 100         | 100 |
| 6   | BX    | 147/150 (98%) | 144 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 7   | BY    | 204/216 (94%) | 199 (98%)  | 5 (2%)  | 0        | 100         | 100 |
| 8   | Ba    | 391/423 (92%) | 379 (97%)  | 12 (3%) | 0        | 100         | 100 |
| 9   | Bb    | 352/380 (93%) | 336 (96%)  | 16 (4%) | 0        | 100         | 100 |
| 10  | Bc    | 293/334 (88%) | 279 (95%)  | 14 (5%) | 0        | 100         | 100 |
| 11  | Bd    | 138/206 (67%) | 133 (96%)  | 5 (4%)  | 0        | 100         | 100 |
| 12  | Be    | 120/135 (89%) | 115 (96%)  | 5 (4%)  | 0        | 100         | 100 |
| 13  | Bf    | 106/142 (75%) | 101 (95%)  | 3 (3%)  | 2 (2%)   | 6           | 32  |
| 14  | Bg    | 146/159 (92%) | 135 (92%)  | 11 (8%) | 0        | 100         | 100 |
| 15  | Bh    | 287/332 (86%) | 274 (96%)  | 13 (4%) | 0        | 100         | 100 |
| 16  | Bi    | 258/306 (84%) | 249 (96%)  | 9 (4%)  | 0        | 100         | 100 |
| 17  | Bj    | 211/279 (76%) | 204 (97%)  | 7 (3%)  | 0        | 100         | 100 |
| 18  | Bk    | 151/269 (56%) | 146 (97%)  | 5 (3%)  | 0        | 100         | 100 |
| 19  | Bl    | 131/166 (79%) | 129 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 20  | Bm    | 107/198 (54%) | 104 (97%)  | 3 (3%)  | 0        | 100         | 100 |
| 21  | Bn    | 95/128 (74%)  | 90 (95%)   | 5 (5%)  | 0        | 100         | 100 |
| 22  | Bo    | 95/124 (77%)  | 93 (98%)   | 2 (2%)  | 0        | 100         | 100 |
| 23  | Bp    | 95/112 (85%)  | 91 (96%)   | 4 (4%)  | 0        | 100         | 100 |
| 24  | Bq    | 83/138 (60%)  | 75 (90%)   | 8 (10%) | 0        | 100         | 100 |
| 25  | Bt    | 92/102 (90%)  | 89 (97%)   | 3 (3%)  | 0        | 100         | 100 |
| 26  | Bu    | 147/205 (72%) | 140 (95%)  | 5 (3%)  | 2 (1%)   | 9           | 39  |
| 27  | Bv    | 133/222 (60%) | 133 (100%) | 0       | 0        | 100         | 100 |
| 28  | B0    | 108/148 (73%) | 106 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 29  | Bw    | 385/433 (89%) | 363 (94%)  | 22 (6%) | 0        | 100         | 100 |
| 30  | Bx    | 160/196 (82%) | 152 (95%)  | 8 (5%)  | 0        | 100         | 100 |
| 32  | AB    | 218/289 (75%) | 210 (96%)  | 8 (4%)  | 0        | 100         | 100 |
| 33  | AC    | 130/167 (78%) | 124 (95%)  | 6 (5%)  | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|---------------|------------|---------|----------|-------------|-----|
| 34  | AE    | 341/430 (79%) | 324 (95%)  | 17 (5%) | 0        | 100         | 100 |
| 35  | AF    | 120/276 (44%) | 115 (96%)  | 5 (4%)  | 0        | 100         | 100 |
| 36  | AG    | 206/242 (85%) | 206 (100%) | 0       | 0        | 100         | 100 |
| 37  | AJ    | 138/200 (69%) | 130 (94%)  | 8 (6%)  | 0        | 100         | 100 |
| 38  | AK    | 135/196 (69%) | 131 (97%)  | 4 (3%)  | 0        | 100         | 100 |
| 39  | AL    | 107/139 (77%) | 102 (95%)  | 5 (5%)  | 0        | 100         | 100 |
| 40  | AN    | 99/128 (77%)  | 98 (99%)   | 1 (1%)  | 0        | 100         | 100 |
| 41  | AO    | 173/239 (72%) | 169 (98%)  | 4 (2%)  | 0        | 100         | 100 |
| 42  | AP    | 115/135 (85%) | 112 (97%)  | 3 (3%)  | 0        | 100         | 100 |
| 43  | AQ    | 110/130 (85%) | 109 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 44  | AR    | 95/143 (66%)  | 95 (100%)  | 0       | 0        | 100         | 100 |
| 45  | AU    | 84/87 (97%)   | 83 (99%)   | 1 (1%)  | 0        | 100         | 100 |
| 48  | AZ    | 16/18 (89%)   | 16 (100%)  | 0       | 0        | 100         | 100 |
| 49  | Aa    | 290/382 (76%) | 286 (99%)  | 4 (1%)  | 0        | 100         | 100 |
| 50  | Ab    | 133/190 (70%) | 131 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 51  | Ac    | 167/173 (96%) | 165 (99%)  | 2 (1%)  | 0        | 100         | 100 |
| 52  | Ad    | 175/205 (85%) | 174 (99%)  | 1 (1%)  | 0        | 100         | 100 |
| 53  | Ae    | 386/455 (85%) | 365 (95%)  | 19 (5%) | 2 (0%)   | 24          | 62  |
| 54  | B1    | 242/256 (94%) | 242 (100%) | 0       | 0        | 100         | 100 |
| 55  | Af    | 97/188 (52%)  | 91 (94%)   | 6 (6%)  | 0        | 100         | 100 |
| 56  | Ag    | 351/410 (86%) | 337 (96%)  | 14 (4%) | 0        | 100         | 100 |
| 57  | Ah    | 118/387 (30%) | 118 (100%) | 0       | 0        | 100         | 100 |
| 58  | Ai    | 97/106 (92%)  | 97 (100%)  | 0       | 0        | 100         | 100 |
| 59  | Aj    | 211/218 (97%) | 205 (97%)  | 6 (3%)  | 0        | 100         | 100 |
| 60  | Ak    | 273/325 (84%) | 267 (98%)  | 6 (2%)  | 0        | 100         | 100 |
| 61  | Am    | 114/118 (97%) | 112 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 62  | An    | 70/199 (35%)  | 69 (99%)   | 1 (1%)  | 0        | 100         | 100 |
| 63  | Ao    | 564/692 (82%) | 552 (98%)  | 12 (2%) | 0        | 100         | 100 |
| 64  | Ap    | 188/258 (73%) | 181 (96%)  | 7 (4%)  | 0        | 100         | 100 |
| 65  | CL    | 43/198 (22%)  | 40 (93%)   | 3 (7%)  | 0        | 100         | 100 |
| 65  | DL    | 25/198 (13%)  | 25 (100%)  | 0       | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Favoured    | Allowed  | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|----------|----------|-------------|-----|
| 65  | EL    | 26/198 (13%)      | 26 (100%)   | 0        | 0        | 100         | 100 |
| 65  | FL    | 25/198 (13%)      | 24 (96%)    | 1 (4%)   | 0        | 100         | 100 |
| 65  | GL    | 25/198 (13%)      | 25 (100%)   | 0        | 0        | 100         | 100 |
| 65  | HL    | 24/198 (12%)      | 24 (100%)   | 0        | 0        | 100         | 100 |
| 65  | LL    | 68/198 (34%)      | 67 (98%)    | 1 (2%)   | 0        | 100         | 100 |
| 66  | B2    | 177/252 (70%)     | 176 (99%)   | 1 (1%)   | 0        | 100         | 100 |
| 67  | B3    | 116/161 (72%)     | 113 (97%)   | 3 (3%)   | 0        | 100         | 100 |
| 68  | B4    | 60/126 (48%)      | 52 (87%)    | 8 (13%)  | 0        | 100         | 100 |
| 69  | B5    | 108/188 (57%)     | 107 (99%)   | 1 (1%)   | 0        | 100         | 100 |
| 70  | B6    | 50/65 (77%)       | 50 (100%)   | 0        | 0        | 100         | 100 |
| 71  | B7    | 44/95 (46%)       | 44 (100%)   | 0        | 0        | 100         | 100 |
| 72  | B8    | 93/188 (50%)      | 91 (98%)    | 2 (2%)   | 0        | 100         | 100 |
| 73  | B9    | 36/100 (36%)      | 36 (100%)   | 0        | 0        | 100         | 100 |
| 75  | BC    | 688/721 (95%)     | 641 (93%)   | 47 (7%)  | 0        | 100         | 100 |
| 76  | BD    | 238/306 (78%)     | 229 (96%)   | 9 (4%)   | 0        | 100         | 100 |
| 77  | BE    | 305/348 (88%)     | 287 (94%)   | 18 (6%)  | 0        | 100         | 100 |
| 78  | BF    | 248/294 (84%)     | 243 (98%)   | 5 (2%)   | 0        | 100         | 100 |
| 79  | BI    | 96/268 (36%)      | 95 (99%)    | 1 (1%)   | 0        | 100         | 100 |
| 80  | BJ    | 210/262 (80%)     | 197 (94%)   | 13 (6%)  | 0        | 100         | 100 |
| 81  | BK    | 174/192 (91%)     | 166 (95%)   | 8 (5%)   | 0        | 100         | 100 |
| 82  | BN    | 175/178 (98%)     | 169 (97%)   | 6 (3%)   | 0        | 100         | 100 |
| 83  | BO    | 113/145 (78%)     | 109 (96%)   | 4 (4%)   | 0        | 100         | 100 |
| 84  | BP    | 286/296 (97%)     | 274 (96%)   | 12 (4%)  | 0        | 100         | 100 |
| 85  | BQ    | 220/251 (88%)     | 216 (98%)   | 4 (2%)   | 0        | 100         | 100 |
| 86  | BR    | 151/169 (89%)     | 144 (95%)   | 7 (5%)   | 0        | 100         | 100 |
| 87  | BS    | 141/180 (78%)     | 130 (92%)   | 11 (8%)  | 0        | 100         | 100 |
| All | All   | 14964/20312 (74%) | 14454 (97%) | 504 (3%) | 6 (0%)   | 100         | 100 |

All (6) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13  | Bf    | 80  | PRO  |
| 26  | Bu    | 167 | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13  | Bf    | 78  | PRO  |
| 53  | Ae    | 342 | PRO  |
| 53  | Ae    | 341 | GLN  |
| 26  | Bu    | 166 | GLU  |

### 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   | AI    | 273/333 (82%) | 272 (100%) | 1 (0%)   | 84          | 82  |
| 2   | BT    | 204/258 (79%) | 200 (98%)  | 4 (2%)   | 48          | 65  |
| 3   | BU    | 118/127 (93%) | 118 (100%) | 0        | 100         | 100 |
| 4   | BV    | 136/178 (76%) | 131 (96%)  | 5 (4%)   | 30          | 51  |
| 5   | BW    | 144/180 (80%) | 144 (100%) | 0        | 100         | 100 |
| 6   | BX    | 116/134 (87%) | 116 (100%) | 0        | 100         | 100 |
| 7   | BY    | 185/192 (96%) | 181 (98%)  | 4 (2%)   | 45          | 64  |
| 8   | Ba    | 348/365 (95%) | 337 (97%)  | 11 (3%)  | 34          | 56  |
| 9   | Bb    | 310/328 (94%) | 306 (99%)  | 4 (1%)   | 61          | 71  |
| 10  | Bc    | 271/299 (91%) | 268 (99%)  | 3 (1%)   | 65          | 73  |
| 11  | Bd    | 129/181 (71%) | 126 (98%)  | 3 (2%)   | 44          | 64  |
| 12  | Be    | 100/108 (93%) | 99 (99%)   | 1 (1%)   | 68          | 75  |
| 13  | Bf    | 80/133 (60%)  | 80 (100%)  | 0        | 100         | 100 |
| 14  | Bg    | 128/136 (94%) | 123 (96%)  | 5 (4%)   | 28          | 50  |
| 15  | Bh    | 251/284 (88%) | 246 (98%)  | 5 (2%)   | 48          | 65  |
| 16  | Bi    | 236/275 (86%) | 230 (98%)  | 6 (2%)   | 42          | 62  |
| 17  | Bj    | 190/242 (78%) | 186 (98%)  | 4 (2%)   | 47          | 65  |
| 18  | Bk    | 135/226 (60%) | 132 (98%)  | 3 (2%)   | 45          | 64  |
| 19  | Bl    | 122/147 (83%) | 119 (98%)  | 3 (2%)   | 42          | 62  |
| 20  | Bm    | 103/178 (58%) | 103 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Rotameric  | Outliers | Percentiles |     |
|-----|-------|---------------|------------|----------|-------------|-----|
| 21  | Bn    | 88/113 (78%)  | 85 (97%)   | 3 (3%)   | 32          | 55  |
| 22  | Bo    | 77/97 (79%)   | 77 (100%)  | 0        | 100         | 100 |
| 23  | Bp    | 79/88 (90%)   | 76 (96%)   | 3 (4%)   | 29          | 51  |
| 24  | Bq    | 70/114 (61%)  | 65 (93%)   | 5 (7%)   | 13          | 36  |
| 25  | Bt    | 75/82 (92%)   | 75 (100%)  | 0        | 100         | 100 |
| 26  | Bu    | 126/177 (71%) | 126 (100%) | 0        | 100         | 100 |
| 27  | Bv    | 115/183 (63%) | 112 (97%)  | 3 (3%)   | 40          | 61  |
| 28  | B0    | 90/115 (78%)  | 87 (97%)   | 3 (3%)   | 33          | 55  |
| 29  | Bw    | 340/373 (91%) | 337 (99%)  | 3 (1%)   | 70          | 75  |
| 30  | Bx    | 149/173 (86%) | 146 (98%)  | 3 (2%)   | 48          | 65  |
| 32  | AB    | 187/233 (80%) | 185 (99%)  | 2 (1%)   | 65          | 73  |
| 33  | AC    | 115/142 (81%) | 114 (99%)  | 1 (1%)   | 70          | 75  |
| 34  | AE    | 282/351 (80%) | 277 (98%)  | 5 (2%)   | 51          | 66  |
| 35  | AF    | 107/210 (51%) | 104 (97%)  | 3 (3%)   | 38          | 59  |
| 36  | AG    | 181/205 (88%) | 178 (98%)  | 3 (2%)   | 53          | 67  |
| 37  | AJ    | 130/180 (72%) | 126 (97%)  | 4 (3%)   | 35          | 56  |
| 38  | AK    | 103/151 (68%) | 102 (99%)  | 1 (1%)   | 68          | 75  |
| 39  | AL    | 92/116 (79%)  | 91 (99%)   | 1 (1%)   | 65          | 73  |
| 40  | AN    | 92/114 (81%)  | 92 (100%)  | 0        | 100         | 100 |
| 41  | AO    | 159/205 (78%) | 158 (99%)  | 1 (1%)   | 78          | 80  |
| 42  | AP    | 97/113 (86%)  | 97 (100%)  | 0        | 100         | 100 |
| 43  | AQ    | 97/114 (85%)  | 96 (99%)   | 1 (1%)   | 68          | 75  |
| 44  | AR    | 89/127 (70%)  | 87 (98%)   | 2 (2%)   | 45          | 64  |
| 45  | AU    | 77/78 (99%)   | 77 (100%)  | 0        | 100         | 100 |
| 49  | Aa    | 258/330 (78%) | 250 (97%)  | 8 (3%)   | 35          | 56  |
| 50  | Ab    | 113/162 (70%) | 113 (100%) | 0        | 100         | 100 |
| 51  | Ac    | 152/155 (98%) | 150 (99%)  | 2 (1%)   | 61          | 71  |
| 52  | Ad    | 149/168 (89%) | 145 (97%)  | 4 (3%)   | 39          | 60  |
| 53  | Ae    | 325/393 (83%) | 319 (98%)  | 6 (2%)   | 51          | 66  |
| 54  | B1    | 219/229 (96%) | 212 (97%)  | 7 (3%)   | 34          | 56  |
| 55  | Af    | 86/160 (54%)  | 83 (96%)   | 3 (4%)   | 32          | 53  |

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| Mol | Chain | Analysed      | Rotameric  | Outliers | Percentiles |     |
|-----|-------|---------------|------------|----------|-------------|-----|
| 56  | Ag    | 312/361 (86%) | 305 (98%)  | 7 (2%)   | 45          | 64  |
| 57  | Ah    | 109/346 (32%) | 109 (100%) | 0        | 100         | 100 |
| 58  | Ai    | 86/93 (92%)   | 85 (99%)   | 1 (1%)   | 63          | 73  |
| 59  | Aj    | 188/190 (99%) | 185 (98%)  | 3 (2%)   | 55          | 69  |
| 60  | Ak    | 249/289 (86%) | 242 (97%)  | 7 (3%)   | 38          | 59  |
| 61  | Am    | 100/102 (98%) | 97 (97%)   | 3 (3%)   | 36          | 57  |
| 62  | An    | 66/174 (38%)  | 66 (100%)  | 0        | 100         | 100 |
| 63  | Ao    | 478/604 (79%) | 463 (97%)  | 15 (3%)  | 35          | 56  |
| 64  | Ap    | 170/225 (76%) | 167 (98%)  | 3 (2%)   | 51          | 66  |
| 65  | CL    | 30/157 (19%)  | 30 (100%)  | 0        | 100         | 100 |
| 65  | DL    | 26/157 (17%)  | 23 (88%)   | 3 (12%)  | 5           | 20  |
| 65  | EL    | 27/157 (17%)  | 27 (100%)  | 0        | 100         | 100 |
| 65  | FL    | 26/157 (17%)  | 26 (100%)  | 0        | 100         | 100 |
| 65  | GL    | 26/157 (17%)  | 25 (96%)   | 1 (4%)   | 29          | 51  |
| 65  | HL    | 25/157 (16%)  | 25 (100%)  | 0        | 100         | 100 |
| 65  | LL    | 59/157 (38%)  | 59 (100%)  | 0        | 100         | 100 |
| 66  | B2    | 164/228 (72%) | 161 (98%)  | 3 (2%)   | 51          | 66  |
| 67  | B3    | 110/150 (73%) | 110 (100%) | 0        | 100         | 100 |
| 68  | B4    | 45/114 (40%)  | 43 (96%)   | 2 (4%)   | 25          | 48  |
| 69  | B5    | 99/163 (61%)  | 97 (98%)   | 2 (2%)   | 48          | 65  |
| 70  | B6    | 49/60 (82%)   | 48 (98%)   | 1 (2%)   | 48          | 65  |
| 71  | B7    | 41/78 (53%)   | 41 (100%)  | 0        | 100         | 100 |
| 72  | B8    | 87/162 (54%)  | 85 (98%)   | 2 (2%)   | 44          | 64  |
| 73  | B9    | 36/77 (47%)   | 35 (97%)   | 1 (3%)   | 38          | 59  |
| 75  | BC    | 589/608 (97%) | 568 (96%)  | 21 (4%)  | 31          | 52  |
| 76  | BD    | 193/248 (78%) | 189 (98%)  | 4 (2%)   | 47          | 65  |
| 77  | BE    | 263/290 (91%) | 259 (98%)  | 4 (2%)   | 57          | 70  |
| 78  | BF    | 217/251 (86%) | 214 (99%)  | 3 (1%)   | 59          | 70  |
| 79  | BI    | 88/228 (39%)  | 86 (98%)   | 2 (2%)   | 44          | 64  |
| 80  | BJ    | 192/230 (84%) | 189 (98%)  | 3 (2%)   | 55          | 69  |
| 81  | BK    | 138/151 (91%) | 130 (94%)  | 8 (6%)   | 18          | 41  |

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| Mol | Chain | Analysed          | Rotameric   | Outliers | Percentiles |     |
|-----|-------|-------------------|-------------|----------|-------------|-----|
| 82  | BN    | 156/157 (99%)     | 156 (100%)  | 0        | 100         | 100 |
| 83  | BO    | 99/123 (80%)      | 99 (100%)   | 0        | 100         | 100 |
| 84  | BP    | 245/249 (98%)     | 241 (98%)   | 4 (2%)   | 55          | 69  |
| 85  | BQ    | 190/210 (90%)     | 187 (98%)   | 3 (2%)   | 55          | 69  |
| 86  | BR    | 132/143 (92%)     | 130 (98%)   | 2 (2%)   | 57          | 70  |
| 87  | BS    | 123/153 (80%)     | 120 (98%)   | 3 (2%)   | 43          | 63  |
| All | All   | 13131/17311 (76%) | 12881 (98%) | 250 (2%) | 49          | 66  |

All (250) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AI    | 94  | GLU  |
| 2   | BT    | 121 | THR  |
| 2   | BT    | 187 | LEU  |
| 2   | BT    | 217 | VAL  |
| 2   | BT    | 252 | GLU  |
| 4   | BV    | 69  | VAL  |
| 4   | BV    | 103 | VAL  |
| 4   | BV    | 113 | THR  |
| 4   | BV    | 146 | THR  |
| 4   | BV    | 153 | LEU  |
| 7   | BY    | 86  | VAL  |
| 7   | BY    | 98  | VAL  |
| 7   | BY    | 184 | GLU  |
| 7   | BY    | 186 | THR  |
| 8   | Ba    | 74  | VAL  |
| 8   | Ba    | 139 | LEU  |
| 8   | Ba    | 147 | ILE  |
| 8   | Ba    | 256 | PHE  |
| 8   | Ba    | 270 | VAL  |
| 8   | Ba    | 273 | VAL  |
| 8   | Ba    | 307 | ASP  |
| 8   | Ba    | 337 | GLU  |
| 8   | Ba    | 341 | VAL  |
| 8   | Ba    | 342 | VAL  |
| 8   | Ba    | 391 | VAL  |
| 9   | Bb    | 179 | VAL  |
| 9   | Bb    | 207 | GLU  |
| 9   | Bb    | 233 | VAL  |
| 9   | Bb    | 324 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10  | Bc    | 56  | THR  |
| 10  | Bc    | 152 | GLU  |
| 10  | Bc    | 283 | LEU  |
| 11  | Bd    | 46  | THR  |
| 11  | Bd    | 106 | LEU  |
| 11  | Bd    | 145 | GLU  |
| 12  | Be    | 60  | VAL  |
| 14  | Bg    | 14  | VAL  |
| 14  | Bg    | 62  | VAL  |
| 14  | Bg    | 75  | VAL  |
| 14  | Bg    | 81  | ASN  |
| 14  | Bg    | 112 | VAL  |
| 15  | Bh    | 148 | LEU  |
| 15  | Bh    | 151 | GLU  |
| 15  | Bh    | 164 | GLU  |
| 15  | Bh    | 191 | LEU  |
| 15  | Bh    | 267 | LEU  |
| 16  | Bi    | 56  | PHE  |
| 16  | Bi    | 143 | ASP  |
| 16  | Bi    | 186 | VAL  |
| 16  | Bi    | 221 | THR  |
| 16  | Bi    | 238 | VAL  |
| 16  | Bi    | 244 | GLU  |
| 17  | Bj    | 47  | LEU  |
| 17  | Bj    | 55  | ARG  |
| 17  | Bj    | 84  | TYR  |
| 17  | Bj    | 265 | LYS  |
| 18  | Bk    | 84  | THR  |
| 18  | Bk    | 175 | HIS  |
| 18  | Bk    | 192 | GLU  |
| 19  | Bl    | 42  | VAL  |
| 19  | Bl    | 64  | GLU  |
| 19  | Bl    | 109 | VAL  |
| 21  | Bn    | 43  | VAL  |
| 21  | Bn    | 44  | VAL  |
| 21  | Bn    | 66  | PHE  |
| 23  | Bp    | 27  | VAL  |
| 23  | Bp    | 67  | LEU  |
| 23  | Bp    | 75  | ILE  |
| 24  | Bq    | 73  | MET  |
| 24  | Bq    | 75  | VAL  |
| 24  | Bq    | 85  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 24  | Bq    | 86  | LEU  |
| 24  | Bq    | 101 | VAL  |
| 27  | Bv    | 88  | GLU  |
| 27  | Bv    | 144 | GLU  |
| 27  | Bv    | 151 | ASP  |
| 28  | B0    | 53  | ILE  |
| 28  | B0    | 117 | VAL  |
| 28  | B0    | 131 | VAL  |
| 29  | Bw    | 47  | ILE  |
| 29  | Bw    | 131 | LEU  |
| 29  | Bw    | 255 | VAL  |
| 30  | Bx    | 43  | ASP  |
| 30  | Bx    | 100 | LEU  |
| 30  | Bx    | 152 | THR  |
| 32  | AB    | 201 | VAL  |
| 32  | AB    | 235 | VAL  |
| 33  | AC    | 52  | THR  |
| 34  | AE    | 181 | ARG  |
| 34  | AE    | 189 | ARG  |
| 34  | AE    | 289 | THR  |
| 34  | AE    | 336 | VAL  |
| 34  | AE    | 401 | VAL  |
| 35  | AF    | 76  | GLU  |
| 35  | AF    | 105 | CYS  |
| 35  | AF    | 106 | GLU  |
| 36  | AG    | 64  | TYR  |
| 36  | AG    | 65  | GLU  |
| 36  | AG    | 208 | GLU  |
| 37  | AJ    | 53  | ASP  |
| 37  | AJ    | 54  | VAL  |
| 37  | AJ    | 97  | LEU  |
| 37  | AJ    | 126 | ILE  |
| 38  | AK    | 68  | ILE  |
| 39  | AL    | 135 | VAL  |
| 41  | AO    | 127 | GLU  |
| 43  | AQ    | 71  | VAL  |
| 44  | AR    | 69  | CYS  |
| 44  | AR    | 77  | ASN  |
| 49  | Aa    | 91  | THR  |
| 49  | Aa    | 129 | THR  |
| 49  | Aa    | 150 | MET  |
| 49  | Aa    | 153 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 49  | Aa    | 196 | VAL  |
| 49  | Aa    | 273 | GLU  |
| 49  | Aa    | 329 | LEU  |
| 49  | Aa    | 373 | GLU  |
| 51  | Ac    | 90  | VAL  |
| 51  | Ac    | 106 | LEU  |
| 52  | Ad    | 29  | THR  |
| 52  | Ad    | 44  | THR  |
| 52  | Ad    | 145 | GLU  |
| 52  | Ad    | 169 | THR  |
| 53  | Ae    | 234 | THR  |
| 53  | Ae    | 235 | ASP  |
| 53  | Ae    | 280 | LEU  |
| 53  | Ae    | 321 | ASP  |
| 53  | Ae    | 360 | VAL  |
| 53  | Ae    | 388 | VAL  |
| 54  | B1    | 6   | VAL  |
| 54  | B1    | 33  | GLU  |
| 54  | B1    | 62  | VAL  |
| 54  | B1    | 126 | THR  |
| 54  | B1    | 160 | ASP  |
| 54  | B1    | 232 | GLU  |
| 54  | B1    | 241 | GLN  |
| 55  | Af    | 109 | VAL  |
| 55  | Af    | 160 | ASP  |
| 55  | Af    | 173 | LEU  |
| 56  | Ag    | 141 | LEU  |
| 56  | Ag    | 208 | VAL  |
| 56  | Ag    | 259 | VAL  |
| 56  | Ag    | 261 | VAL  |
| 56  | Ag    | 306 | VAL  |
| 56  | Ag    | 336 | LEU  |
| 56  | Ag    | 368 | GLU  |
| 58  | Ai    | 85  | LEU  |
| 59  | Aj    | 40  | THR  |
| 59  | Aj    | 107 | GLU  |
| 59  | Aj    | 154 | THR  |
| 60  | Ak    | 93  | VAL  |
| 60  | Ak    | 165 | ILE  |
| 60  | Ak    | 177 | VAL  |
| 60  | Ak    | 227 | LEU  |
| 60  | Ak    | 246 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 60  | Ak    | 252 | GLU  |
| 60  | Ak    | 308 | GLU  |
| 61  | Am    | 40  | LYS  |
| 61  | Am    | 66  | CYS  |
| 61  | Am    | 95  | GLU  |
| 63  | Ao    | 78  | VAL  |
| 63  | Ao    | 146 | GLU  |
| 63  | Ao    | 294 | VAL  |
| 63  | Ao    | 314 | GLU  |
| 63  | Ao    | 349 | TYR  |
| 63  | Ao    | 381 | LEU  |
| 63  | Ao    | 429 | LEU  |
| 63  | Ao    | 489 | PHE  |
| 63  | Ao    | 533 | GLU  |
| 63  | Ao    | 537 | LEU  |
| 63  | Ao    | 546 | GLU  |
| 63  | Ao    | 563 | GLU  |
| 63  | Ao    | 612 | GLU  |
| 63  | Ao    | 644 | VAL  |
| 63  | Ao    | 646 | GLU  |
| 64  | Ap    | 115 | VAL  |
| 64  | Ap    | 179 | THR  |
| 64  | Ap    | 233 | GLU  |
| 65  | DL    | 66  | GLN  |
| 65  | DL    | 79  | ILE  |
| 65  | DL    | 84  | GLU  |
| 65  | GL    | 81  | ASP  |
| 66  | B2    | 92  | LEU  |
| 66  | B2    | 228 | LEU  |
| 66  | B2    | 238 | GLU  |
| 68  | B4    | 48  | THR  |
| 68  | B4    | 58  | VAL  |
| 69  | B5    | 103 | VAL  |
| 69  | B5    | 153 | THR  |
| 70  | B6    | 16  | ILE  |
| 72  | B8    | 137 | THR  |
| 72  | B8    | 163 | THR  |
| 73  | B9    | 65  | THR  |
| 75  | BC    | 151 | VAL  |
| 75  | BC    | 203 | ILE  |
| 75  | BC    | 205 | MET  |
| 75  | BC    | 228 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 75  | BC    | 237 | GLU  |
| 75  | BC    | 242 | LEU  |
| 75  | BC    | 268 | PHE  |
| 75  | BC    | 269 | LEU  |
| 75  | BC    | 297 | LEU  |
| 75  | BC    | 314 | LEU  |
| 75  | BC    | 325 | ASN  |
| 75  | BC    | 328 | ILE  |
| 75  | BC    | 485 | ASP  |
| 75  | BC    | 533 | VAL  |
| 75  | BC    | 559 | LEU  |
| 75  | BC    | 562 | GLU  |
| 75  | BC    | 578 | ILE  |
| 75  | BC    | 616 | HIS  |
| 75  | BC    | 624 | ILE  |
| 75  | BC    | 636 | GLN  |
| 75  | BC    | 681 | VAL  |
| 76  | BD    | 190 | VAL  |
| 76  | BD    | 208 | ILE  |
| 76  | BD    | 216 | VAL  |
| 76  | BD    | 240 | THR  |
| 77  | BE    | 111 | THR  |
| 77  | BE    | 236 | THR  |
| 77  | BE    | 245 | THR  |
| 77  | BE    | 273 | VAL  |
| 78  | BF    | 47  | VAL  |
| 78  | BF    | 120 | VAL  |
| 78  | BF    | 262 | THR  |
| 79  | BI    | 64  | LEU  |
| 79  | BI    | 107 | VAL  |
| 80  | BJ    | 39  | VAL  |
| 80  | BJ    | 78  | LEU  |
| 80  | BJ    | 161 | VAL  |
| 81  | BK    | 24  | VAL  |
| 81  | BK    | 52  | GLU  |
| 81  | BK    | 62  | GLU  |
| 81  | BK    | 66  | LEU  |
| 81  | BK    | 111 | LEU  |
| 81  | BK    | 119 | GLU  |
| 81  | BK    | 124 | LYS  |
| 81  | BK    | 157 | LYS  |
| 84  | BP    | 61  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 84  | BP    | 155 | GLU  |
| 84  | BP    | 215 | THR  |
| 84  | BP    | 286 | THR  |
| 85  | BQ    | 56  | VAL  |
| 85  | BQ    | 175 | PHE  |
| 85  | BQ    | 177 | ASP  |
| 86  | BR    | 65  | LEU  |
| 86  | BR    | 144 | THR  |
| 87  | BS    | 68  | TRP  |
| 87  | BS    | 107 | THR  |
| 87  | BS    | 141 | ILE  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (298) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AI    | 101 | GLN  |
| 1   | AI    | 139 | GLN  |
| 1   | AI    | 156 | GLN  |
| 1   | AI    | 163 | HIS  |
| 1   | AI    | 252 | GLN  |
| 1   | AI    | 319 | HIS  |
| 2   | BT    | 139 | GLN  |
| 2   | BT    | 158 | GLN  |
| 2   | BT    | 172 | GLN  |
| 2   | BT    | 213 | GLN  |
| 2   | BT    | 219 | GLN  |
| 3   | BU    | 27  | HIS  |
| 3   | BU    | 79  | HIS  |
| 3   | BU    | 89  | ASN  |
| 4   | BV    | 109 | GLN  |
| 4   | BV    | 122 | ASN  |
| 5   | BW    | 73  | HIS  |
| 5   | BW    | 113 | GLN  |
| 5   | BW    | 208 | HIS  |
| 6   | BX    | 4   | ASN  |
| 6   | BX    | 35  | GLN  |
| 6   | BX    | 98  | GLN  |
| 7   | BY    | 18  | ASN  |
| 7   | BY    | 35  | ASN  |
| 7   | BY    | 84  | ASN  |
| 8   | Ba    | 108 | HIS  |
| 8   | Ba    | 119 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8   | Ba    | 149 | ASN  |
| 8   | Ba    | 205 | GLN  |
| 8   | Ba    | 221 | GLN  |
| 8   | Ba    | 223 | HIS  |
| 8   | Ba    | 266 | GLN  |
| 8   | Ba    | 289 | HIS  |
| 8   | Ba    | 324 | GLN  |
| 8   | Ba    | 331 | ASN  |
| 8   | Ba    | 360 | ASN  |
| 9   | Bb    | 63  | GLN  |
| 9   | Bb    | 220 | ASN  |
| 9   | Bb    | 308 | GLN  |
| 9   | Bb    | 354 | GLN  |
| 9   | Bb    | 373 | HIS  |
| 10  | Bc    | 46  | ASN  |
| 10  | Bc    | 243 | GLN  |
| 10  | Bc    | 294 | GLN  |
| 10  | Bc    | 310 | ASN  |
| 11  | Bd    | 18  | GLN  |
| 11  | Bd    | 36  | GLN  |
| 11  | Bd    | 114 | HIS  |
| 12  | Be    | 127 | GLN  |
| 14  | Bg    | 17  | ASN  |
| 14  | Bg    | 127 | GLN  |
| 14  | Bg    | 135 | ASN  |
| 15  | Bh    | 42  | GLN  |
| 15  | Bh    | 69  | HIS  |
| 15  | Bh    | 106 | GLN  |
| 15  | Bh    | 177 | GLN  |
| 15  | Bh    | 222 | GLN  |
| 16  | Bi    | 47  | GLN  |
| 16  | Bi    | 193 | GLN  |
| 16  | Bi    | 286 | GLN  |
| 17  | Bj    | 87  | HIS  |
| 17  | Bj    | 97  | GLN  |
| 18  | Bk    | 138 | GLN  |
| 18  | Bk    | 158 | GLN  |
| 18  | Bk    | 177 | ASN  |
| 20  | Bm    | 68  | GLN  |
| 20  | Bm    | 107 | ASN  |
| 20  | Bm    | 151 | HIS  |
| 21  | Bn    | 33  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 21  | Bn    | 120 | HIS  |
| 21  | Bn    | 122 | ASN  |
| 22  | Bo    | 31  | GLN  |
| 22  | Bo    | 69  | GLN  |
| 22  | Bo    | 100 | GLN  |
| 23  | Bp    | 15  | GLN  |
| 23  | Bp    | 35  | GLN  |
| 23  | Bp    | 93  | HIS  |
| 24  | Bq    | 71  | HIS  |
| 25  | Bt    | 30  | GLN  |
| 25  | Bt    | 34  | ASN  |
| 25  | Bt    | 91  | GLN  |
| 26  | Bu    | 67  | GLN  |
| 26  | Bu    | 145 | ASN  |
| 27  | Bv    | 107 | GLN  |
| 27  | Bv    | 112 | GLN  |
| 27  | Bv    | 138 | GLN  |
| 28  | B0    | 76  | HIS  |
| 28  | B0    | 107 | ASN  |
| 29  | Bw    | 67  | GLN  |
| 29  | Bw    | 87  | GLN  |
| 29  | Bw    | 104 | ASN  |
| 29  | Bw    | 186 | ASN  |
| 29  | Bw    | 226 | GLN  |
| 29  | Bw    | 228 | ASN  |
| 29  | Bw    | 352 | GLN  |
| 29  | Bw    | 381 | ASN  |
| 29  | Bw    | 385 | ASN  |
| 29  | Bw    | 402 | ASN  |
| 29  | Bw    | 414 | GLN  |
| 30  | Bx    | 130 | ASN  |
| 30  | Bx    | 164 | ASN  |
| 32  | AB    | 119 | GLN  |
| 32  | AB    | 147 | HIS  |
| 32  | AB    | 149 | GLN  |
| 33  | AC    | 126 | GLN  |
| 33  | AC    | 154 | HIS  |
| 34  | AE    | 175 | GLN  |
| 34  | AE    | 288 | HIS  |
| 34  | AE    | 292 | HIS  |
| 34  | AE    | 308 | GLN  |
| 34  | AE    | 317 | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 34  | AE    | 356 | GLN  |
| 34  | AE    | 360 | GLN  |
| 34  | AE    | 369 | HIS  |
| 35  | AF    | 92  | ASN  |
| 36  | AG    | 45  | GLN  |
| 36  | AG    | 127 | HIS  |
| 36  | AG    | 140 | ASN  |
| 36  | AG    | 196 | HIS  |
| 36  | AG    | 215 | ASN  |
| 36  | AG    | 233 | ASN  |
| 37  | AJ    | 125 | HIS  |
| 37  | AJ    | 183 | HIS  |
| 38  | AK    | 73  | ASN  |
| 38  | AK    | 121 | ASN  |
| 38  | AK    | 131 | GLN  |
| 38  | AK    | 185 | HIS  |
| 38  | AK    | 186 | ASN  |
| 39  | AL    | 35  | GLN  |
| 39  | AL    | 74  | ASN  |
| 39  | AL    | 77  | ASN  |
| 39  | AL    | 134 | HIS  |
| 40  | AN    | 113 | HIS  |
| 40  | AN    | 117 | HIS  |
| 40  | AN    | 124 | GLN  |
| 41  | AO    | 84  | HIS  |
| 41  | AO    | 147 | HIS  |
| 42  | AP    | 28  | ASN  |
| 42  | AP    | 123 | GLN  |
| 43  | AQ    | 23  | GLN  |
| 43  | AQ    | 52  | HIS  |
| 49  | Aa    | 189 | HIS  |
| 49  | Aa    | 251 | ASN  |
| 49  | Aa    | 289 | HIS  |
| 49  | Aa    | 348 | HIS  |
| 49  | Aa    | 369 | GLN  |
| 49  | Aa    | 372 | GLN  |
| 50  | Ab    | 66  | HIS  |
| 51  | Ac    | 51  | ASN  |
| 51  | Ac    | 56  | GLN  |
| 51  | Ac    | 63  | GLN  |
| 51  | Ac    | 95  | ASN  |
| 51  | Ac    | 118 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 51  | Ac    | 122 | GLN  |
| 51  | Ac    | 125 | HIS  |
| 52  | Ad    | 62  | GLN  |
| 52  | Ad    | 102 | HIS  |
| 52  | Ad    | 109 | ASN  |
| 52  | Ad    | 135 | GLN  |
| 52  | Ad    | 159 | GLN  |
| 52  | Ad    | 188 | ASN  |
| 53  | Ae    | 118 | ASN  |
| 53  | Ae    | 140 | ASN  |
| 53  | Ae    | 181 | ASN  |
| 53  | Ae    | 278 | GLN  |
| 53  | Ae    | 421 | GLN  |
| 54  | B1    | 4   | HIS  |
| 54  | B1    | 27  | HIS  |
| 54  | B1    | 70  | HIS  |
| 54  | B1    | 172 | GLN  |
| 56  | Ag    | 61  | GLN  |
| 56  | Ag    | 65  | GLN  |
| 56  | Ag    | 68  | ASN  |
| 56  | Ag    | 94  | ASN  |
| 56  | Ag    | 113 | ASN  |
| 56  | Ag    | 147 | GLN  |
| 56  | Ag    | 148 | ASN  |
| 56  | Ag    | 179 | GLN  |
| 56  | Ag    | 200 | GLN  |
| 56  | Ag    | 204 | GLN  |
| 56  | Ag    | 311 | GLN  |
| 56  | Ag    | 325 | GLN  |
| 56  | Ag    | 362 | ASN  |
| 56  | Ag    | 363 | ASN  |
| 56  | Ag    | 386 | ASN  |
| 56  | Ag    | 389 | GLN  |
| 57  | Ah    | 309 | ASN  |
| 57  | Ah    | 331 | GLN  |
| 57  | Ah    | 364 | HIS  |
| 57  | Ah    | 370 | ASN  |
| 59  | Aj    | 88  | GLN  |
| 59  | Aj    | 177 | GLN  |
| 60  | Ak    | 66  | GLN  |
| 60  | Ak    | 263 | ASN  |
| 60  | Ak    | 270 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 60  | Ak    | 303 | ASN  |
| 60  | Ak    | 307 | ASN  |
| 61  | Am    | 113 | ASN  |
| 61  | Am    | 116 | HIS  |
| 63  | Ao    | 104 | HIS  |
| 63  | Ao    | 158 | GLN  |
| 63  | Ao    | 260 | HIS  |
| 63  | Ao    | 280 | ASN  |
| 63  | Ao    | 329 | GLN  |
| 63  | Ao    | 336 | GLN  |
| 63  | Ao    | 473 | GLN  |
| 63  | Ao    | 542 | GLN  |
| 63  | Ao    | 543 | HIS  |
| 63  | Ao    | 593 | GLN  |
| 64  | Ap    | 81  | HIS  |
| 64  | Ap    | 98  | ASN  |
| 64  | Ap    | 152 | GLN  |
| 64  | Ap    | 160 | HIS  |
| 64  | Ap    | 181 | HIS  |
| 64  | Ap    | 221 | GLN  |
| 65  | CL    | 66  | GLN  |
| 65  | DL    | 65  | GLN  |
| 65  | DL    | 66  | GLN  |
| 65  | DL    | 83  | ASN  |
| 65  | FL    | 65  | GLN  |
| 65  | FL    | 83  | ASN  |
| 65  | GL    | 83  | ASN  |
| 65  | LL    | 154 | GLN  |
| 66  | B2    | 90  | GLN  |
| 66  | B2    | 218 | GLN  |
| 66  | B2    | 242 | HIS  |
| 69  | B5    | 83  | ASN  |
| 69  | B5    | 90  | ASN  |
| 69  | B5    | 120 | HIS  |
| 69  | B5    | 144 | GLN  |
| 69  | B5    | 188 | ASN  |
| 70  | B6    | 23  | GLN  |
| 72  | B8    | 118 | HIS  |
| 75  | BC    | 124 | HIS  |
| 75  | BC    | 154 | GLN  |
| 75  | BC    | 161 | GLN  |
| 75  | BC    | 330 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 75  | BC    | 344 | ASN  |
| 75  | BC    | 349 | ASN  |
| 75  | BC    | 488 | ASN  |
| 75  | BC    | 539 | HIS  |
| 75  | BC    | 577 | ASN  |
| 75  | BC    | 616 | HIS  |
| 75  | BC    | 617 | HIS  |
| 75  | BC    | 636 | GLN  |
| 75  | BC    | 658 | ASN  |
| 75  | BC    | 661 | GLN  |
| 75  | BC    | 669 | ASN  |
| 75  | BC    | 694 | ASN  |
| 75  | BC    | 733 | ASN  |
| 76  | BD    | 116 | HIS  |
| 76  | BD    | 166 | ASN  |
| 76  | BD    | 183 | HIS  |
| 76  | BD    | 228 | GLN  |
| 77  | BE    | 52  | HIS  |
| 77  | BE    | 69  | ASN  |
| 77  | BE    | 128 | HIS  |
| 77  | BE    | 154 | HIS  |
| 77  | BE    | 174 | GLN  |
| 77  | BE    | 281 | ASN  |
| 77  | BE    | 313 | ASN  |
| 77  | BE    | 336 | ASN  |
| 78  | BF    | 74  | GLN  |
| 78  | BF    | 83  | HIS  |
| 78  | BF    | 97  | HIS  |
| 78  | BF    | 251 | HIS  |
| 79  | BI    | 121 | ASN  |
| 79  | BI    | 126 | GLN  |
| 79  | BI    | 136 | ASN  |
| 79  | BI    | 148 | GLN  |
| 80  | BJ    | 41  | HIS  |
| 80  | BJ    | 119 | HIS  |
| 80  | BJ    | 151 | ASN  |
| 80  | BJ    | 189 | GLN  |
| 80  | BJ    | 223 | GLN  |
| 80  | BJ    | 239 | GLN  |
| 81  | BK    | 28  | GLN  |
| 81  | BK    | 133 | GLN  |
| 82  | BN    | 10  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 82  | BN    | 48  | HIS  |
| 82  | BN    | 89  | GLN  |
| 82  | BN    | 140 | ASN  |
| 83  | BO    | 52  | HIS  |
| 83  | BO    | 89  | HIS  |
| 83  | BO    | 103 | ASN  |
| 83  | BO    | 113 | ASN  |
| 83  | BO    | 142 | GLN  |
| 84  | BP    | 94  | GLN  |
| 84  | BP    | 153 | ASN  |
| 85  | BQ    | 68  | ASN  |
| 85  | BQ    | 98  | HIS  |
| 85  | BQ    | 202 | GLN  |
| 85  | BQ    | 210 | GLN  |
| 85  | BQ    | 222 | ASN  |
| 86  | BR    | 100 | GLN  |
| 86  | BR    | 148 | GLN  |
| 87  | BS    | 88  | HIS  |
| 87  | BS    | 142 | ASN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 31  | AA    | 959/16770 (5%)  | 182 (18%)         | 2 (0%)          |
| 31  | BA    | 1542/16770 (9%) | 410 (26%)         | 1 (0%)          |
| 46  | AV    | 70/71 (98%)     | 20 (28%)          | 0               |
| 46  | AY    | 70/71 (98%)     | 24 (34%)          | 1 (1%)          |
| 47  | AX    | 5/6 (83%)       | 0                 | 0               |
| 74  | BB    | 64/73 (87%)     | 18 (28%)          | 0               |
| All | All   | 2710/33761 (8%) | 654 (24%)         | 4 (0%)          |

All (654) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 31  | AA    | 5   | A    |
| 31  | AA    | 10  | U    |
| 31  | AA    | 27  | U    |
| 31  | AA    | 34  | U    |
| 31  | AA    | 42  | A    |
| 31  | AA    | 43  | U    |
| 31  | AA    | 54  | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 31  | AA    | 58  | U    |
| 31  | AA    | 63  | G    |
| 31  | AA    | 65  | C    |
| 31  | AA    | 75  | A    |
| 31  | AA    | 81  | U    |
| 31  | AA    | 83  | C    |
| 31  | AA    | 102 | G    |
| 31  | AA    | 115 | A    |
| 31  | AA    | 120 | A    |
| 31  | AA    | 127 | A    |
| 31  | AA    | 139 | A    |
| 31  | AA    | 147 | G    |
| 31  | AA    | 152 | A    |
| 31  | AA    | 161 | C    |
| 31  | AA    | 164 | C    |
| 31  | AA    | 165 | G    |
| 31  | AA    | 168 | A    |
| 31  | AA    | 170 | A    |
| 31  | AA    | 171 | C    |
| 31  | AA    | 173 | G    |
| 31  | AA    | 175 | A    |
| 31  | AA    | 186 | U    |
| 31  | AA    | 190 | G    |
| 31  | AA    | 191 | C    |
| 31  | AA    | 192 | C    |
| 31  | AA    | 203 | G    |
| 31  | AA    | 212 | A    |
| 31  | AA    | 216 | A    |
| 31  | AA    | 217 | U    |
| 31  | AA    | 222 | A    |
| 31  | AA    | 223 | U    |
| 31  | AA    | 224 | U    |
| 31  | AA    | 231 | G    |
| 31  | AA    | 235 | A    |
| 31  | AA    | 238 | C    |
| 31  | AA    | 244 | C    |
| 31  | AA    | 247 | G    |
| 31  | AA    | 253 | G    |
| 31  | AA    | 256 | G    |
| 31  | AA    | 257 | U    |
| 31  | AA    | 259 | A    |
| 31  | AA    | 273 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 31  | AA    | 281 | G    |
| 31  | AA    | 287 | C    |
| 31  | AA    | 294 | A    |
| 31  | AA    | 296 | G    |
| 31  | AA    | 297 | A    |
| 31  | AA    | 308 | A    |
| 31  | AA    | 309 | A    |
| 31  | AA    | 310 | A    |
| 31  | AA    | 314 | A    |
| 31  | AA    | 315 | U    |
| 31  | AA    | 316 | C    |
| 31  | AA    | 317 | A    |
| 31  | AA    | 320 | A    |
| 31  | AA    | 328 | A    |
| 31  | AA    | 337 | C    |
| 31  | AA    | 345 | U    |
| 31  | AA    | 354 | C    |
| 31  | AA    | 361 | A    |
| 31  | AA    | 362 | A    |
| 31  | AA    | 368 | A    |
| 31  | AA    | 372 | C    |
| 31  | AA    | 395 | C    |
| 31  | AA    | 399 | A    |
| 31  | AA    | 407 | U    |
| 31  | AA    | 417 | C    |
| 31  | AA    | 421 | A    |
| 31  | AA    | 433 | U    |
| 31  | AA    | 450 | C    |
| 31  | AA    | 455 | A    |
| 31  | AA    | 456 | A    |
| 31  | AA    | 457 | C    |
| 31  | AA    | 458 | C    |
| 31  | AA    | 461 | A    |
| 31  | AA    | 464 | A    |
| 31  | AA    | 465 | G    |
| 31  | AA    | 471 | U    |
| 31  | AA    | 472 | A    |
| 31  | AA    | 477 | A    |
| 31  | AA    | 479 | C    |
| 31  | AA    | 494 | C    |
| 31  | AA    | 498 | U    |
| 31  | AA    | 502 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 31  | AA    | 503 | A    |
| 31  | AA    | 518 | A    |
| 31  | AA    | 531 | U    |
| 31  | AA    | 532 | G    |
| 31  | AA    | 538 | C    |
| 31  | AA    | 539 | A    |
| 31  | AA    | 540 | U    |
| 31  | AA    | 541 | C    |
| 31  | AA    | 561 | U    |
| 31  | AA    | 566 | U    |
| 31  | AA    | 571 | A    |
| 31  | AA    | 574 | C    |
| 31  | AA    | 576 | C    |
| 31  | AA    | 587 | U    |
| 31  | AA    | 589 | C    |
| 31  | AA    | 592 | A    |
| 31  | AA    | 593 | C    |
| 31  | AA    | 596 | U    |
| 31  | AA    | 597 | U    |
| 31  | AA    | 604 | U    |
| 31  | AA    | 616 | C    |
| 31  | AA    | 618 | G    |
| 31  | AA    | 619 | C    |
| 31  | AA    | 620 | C    |
| 31  | AA    | 625 | U    |
| 31  | AA    | 626 | C    |
| 31  | AA    | 639 | A    |
| 31  | AA    | 640 | A    |
| 31  | AA    | 641 | A    |
| 31  | AA    | 644 | A    |
| 31  | AA    | 645 | A    |
| 31  | AA    | 646 | C    |
| 31  | AA    | 647 | A    |
| 31  | AA    | 649 | U    |
| 31  | AA    | 650 | A    |
| 31  | AA    | 653 | A    |
| 31  | AA    | 665 | A    |
| 31  | AA    | 681 | A    |
| 31  | AA    | 682 | G    |
| 31  | AA    | 698 | A    |
| 31  | AA    | 699 | U    |
| 31  | AA    | 707 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 31  | AA    | 708 | A    |
| 31  | AA    | 709 | A    |
| 31  | AA    | 711 | A    |
| 31  | AA    | 720 | A    |
| 31  | AA    | 722 | A    |
| 31  | AA    | 731 | A    |
| 31  | AA    | 732 | U    |
| 31  | AA    | 739 | A    |
| 31  | AA    | 743 | A    |
| 31  | AA    | 746 | A    |
| 31  | AA    | 775 | A    |
| 31  | AA    | 782 | G    |
| 31  | AA    | 783 | A    |
| 31  | AA    | 790 | A    |
| 31  | AA    | 791 | G    |
| 31  | AA    | 802 | A    |
| 31  | AA    | 803 | U    |
| 31  | AA    | 806 | A    |
| 31  | AA    | 807 | G    |
| 31  | AA    | 808 | U    |
| 31  | AA    | 822 | A    |
| 31  | AA    | 826 | C    |
| 31  | AA    | 838 | A    |
| 31  | AA    | 841 | C    |
| 31  | AA    | 842 | A    |
| 31  | AA    | 863 | G    |
| 31  | AA    | 865 | A    |
| 31  | AA    | 869 | A    |
| 31  | AA    | 876 | A    |
| 31  | AA    | 877 | A    |
| 31  | AA    | 883 | C    |
| 31  | AA    | 884 | C    |
| 31  | AA    | 885 | U    |
| 31  | AA    | 886 | A    |
| 31  | AA    | 893 | A    |
| 31  | AA    | 894 | U    |
| 31  | AA    | 902 | C    |
| 31  | AA    | 910 | G    |
| 31  | AA    | 918 | A    |
| 31  | AA    | 919 | A    |
| 31  | AA    | 925 | A    |
| 31  | AA    | 928 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 31  | AA    | 930 | G    |
| 31  | AA    | 932 | U    |
| 31  | AA    | 943 | G    |
| 31  | AA    | 946 | A    |
| 31  | AA    | 955 | G    |
| 31  | AA    | 956 | G    |
| 31  | AA    | 959 | U    |
| 46  | AV    | 6   | G    |
| 46  | AV    | 9   | C    |
| 46  | AV    | 14  | A    |
| 46  | AV    | 16  | A    |
| 46  | AV    | 17  | U    |
| 46  | AV    | 18  | A    |
| 46  | AV    | 43  | A    |
| 46  | AV    | 44  | U    |
| 46  | AV    | 45  | G    |
| 46  | AV    | 51  | U    |
| 46  | AV    | 54  | A    |
| 46  | AV    | 55  | C    |
| 46  | AV    | 56  | C    |
| 46  | AV    | 58  | U    |
| 46  | AV    | 60  | C    |
| 46  | AV    | 62  | C    |
| 46  | AV    | 63  | G    |
| 46  | AV    | 64  | U    |
| 46  | AV    | 65  | A    |
| 46  | AV    | 71  | A    |
| 46  | AY    | 6   | G    |
| 46  | AY    | 8   | U    |
| 46  | AY    | 9   | C    |
| 46  | AY    | 12  | C    |
| 46  | AY    | 14  | A    |
| 46  | AY    | 16  | A    |
| 46  | AY    | 17  | U    |
| 46  | AY    | 18  | A    |
| 46  | AY    | 27  | G    |
| 46  | AY    | 43  | A    |
| 46  | AY    | 45  | G    |
| 46  | AY    | 50  | U    |
| 46  | AY    | 53  | U    |
| 46  | AY    | 54  | A    |
| 46  | AY    | 55  | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 46  | AY    | 56  | C    |
| 46  | AY    | 58  | U    |
| 46  | AY    | 60  | C    |
| 46  | AY    | 62  | C    |
| 46  | AY    | 63  | G    |
| 46  | AY    | 64  | U    |
| 46  | AY    | 65  | A    |
| 46  | AY    | 70  | C    |
| 46  | AY    | 71  | A    |
| 31  | BA    | 4   | A    |
| 31  | BA    | 7   | G    |
| 31  | BA    | 11  | G    |
| 31  | BA    | 15  | A    |
| 31  | BA    | 19  | U    |
| 31  | BA    | 20  | A    |
| 31  | BA    | 21  | C    |
| 31  | BA    | 22  | U    |
| 31  | BA    | 26  | C    |
| 31  | BA    | 30  | U    |
| 31  | BA    | 31  | A    |
| 31  | BA    | 32  | C    |
| 31  | BA    | 36  | A    |
| 31  | BA    | 40  | C    |
| 31  | BA    | 42  | C    |
| 31  | BA    | 43  | C    |
| 31  | BA    | 44  | A    |
| 31  | BA    | 45  | A    |
| 31  | BA    | 46  | A    |
| 31  | BA    | 49  | A    |
| 31  | BA    | 51  | A    |
| 31  | BA    | 56  | A    |
| 31  | BA    | 57  | A    |
| 31  | BA    | 59  | A    |
| 31  | BA    | 60  | U    |
| 31  | BA    | 63  | A    |
| 31  | BA    | 66  | U    |
| 31  | BA    | 67  | A    |
| 31  | BA    | 68  | A    |
| 31  | BA    | 82  | G    |
| 31  | BA    | 83  | A    |
| 31  | BA    | 96  | U    |
| 31  | BA    | 97  | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 31  | BA    | 104 | C    |
| 31  | BA    | 105 | G    |
| 31  | BA    | 109 | U    |
| 31  | BA    | 112 | A    |
| 31  | BA    | 115 | U    |
| 31  | BA    | 119 | A    |
| 31  | BA    | 125 | A    |
| 31  | BA    | 129 | A    |
| 31  | BA    | 132 | G    |
| 31  | BA    | 139 | G    |
| 31  | BA    | 140 | A    |
| 31  | BA    | 141 | A    |
| 31  | BA    | 142 | U    |
| 31  | BA    | 143 | A    |
| 31  | BA    | 146 | A    |
| 31  | BA    | 147 | U    |
| 31  | BA    | 163 | C    |
| 31  | BA    | 164 | A    |
| 31  | BA    | 168 | A    |
| 31  | BA    | 172 | C    |
| 31  | BA    | 178 | C    |
| 31  | BA    | 180 | A    |
| 31  | BA    | 182 | C    |
| 31  | BA    | 188 | C    |
| 31  | BA    | 190 | U    |
| 31  | BA    | 192 | A    |
| 31  | BA    | 205 | A    |
| 31  | BA    | 218 | A    |
| 31  | BA    | 219 | A    |
| 31  | BA    | 223 | A    |
| 31  | BA    | 225 | C    |
| 31  | BA    | 229 | A    |
| 31  | BA    | 231 | C    |
| 31  | BA    | 237 | A    |
| 31  | BA    | 238 | C    |
| 31  | BA    | 239 | C    |
| 31  | BA    | 243 | A    |
| 31  | BA    | 245 | A    |
| 31  | BA    | 254 | G    |
| 31  | BA    | 263 | G    |
| 31  | BA    | 265 | G    |
| 31  | BA    | 271 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 31  | BA    | 272 | A    |
| 31  | BA    | 273 | A    |
| 31  | BA    | 275 | A    |
| 31  | BA    | 277 | A    |
| 31  | BA    | 295 | G    |
| 31  | BA    | 309 | A    |
| 31  | BA    | 311 | A    |
| 31  | BA    | 313 | U    |
| 31  | BA    | 322 | G    |
| 31  | BA    | 324 | G    |
| 31  | BA    | 329 | A    |
| 31  | BA    | 330 | A    |
| 31  | BA    | 331 | A    |
| 31  | BA    | 337 | A    |
| 31  | BA    | 338 | C    |
| 31  | BA    | 339 | G    |
| 31  | BA    | 340 | A    |
| 31  | BA    | 351 | A    |
| 31  | BA    | 352 | G    |
| 31  | BA    | 359 | G    |
| 31  | BA    | 366 | A    |
| 31  | BA    | 368 | A    |
| 31  | BA    | 369 | G    |
| 31  | BA    | 371 | A    |
| 31  | BA    | 373 | U    |
| 31  | BA    | 374 | U    |
| 31  | BA    | 376 | A    |
| 31  | BA    | 390 | A    |
| 31  | BA    | 393 | A    |
| 31  | BA    | 394 | C    |
| 31  | BA    | 398 | A    |
| 31  | BA    | 406 | U    |
| 31  | BA    | 409 | A    |
| 31  | BA    | 413 | C    |
| 31  | BA    | 414 | A    |
| 31  | BA    | 427 | G    |
| 31  | BA    | 428 | A    |
| 31  | BA    | 429 | G    |
| 31  | BA    | 433 | G    |
| 31  | BA    | 434 | U    |
| 31  | BA    | 435 | C    |
| 31  | BA    | 446 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 31  | BA    | 447 | A    |
| 31  | BA    | 448 | G    |
| 31  | BA    | 449 | C    |
| 31  | BA    | 459 | A    |
| 31  | BA    | 460 | C    |
| 31  | BA    | 467 | A    |
| 31  | BA    | 468 | A    |
| 31  | BA    | 472 | U    |
| 31  | BA    | 473 | G    |
| 31  | BA    | 474 | A    |
| 31  | BA    | 479 | A    |
| 31  | BA    | 480 | G    |
| 31  | BA    | 490 | U    |
| 31  | BA    | 491 | U    |
| 31  | BA    | 492 | A    |
| 31  | BA    | 493 | A    |
| 31  | BA    | 494 | U    |
| 31  | BA    | 497 | U    |
| 31  | BA    | 498 | A    |
| 31  | BA    | 499 | C    |
| 31  | BA    | 500 | C    |
| 31  | BA    | 501 | A    |
| 31  | BA    | 503 | A    |
| 31  | BA    | 504 | G    |
| 31  | BA    | 505 | U    |
| 31  | BA    | 509 | C    |
| 31  | BA    | 514 | A    |
| 31  | BA    | 515 | A    |
| 31  | BA    | 516 | G    |
| 31  | BA    | 517 | C    |
| 31  | BA    | 518 | A    |
| 31  | BA    | 530 | A    |
| 31  | BA    | 531 | G    |
| 31  | BA    | 532 | A    |
| 31  | BA    | 533 | A    |
| 31  | BA    | 541 | A    |
| 31  | BA    | 545 | U    |
| 31  | BA    | 547 | A    |
| 31  | BA    | 548 | A    |
| 31  | BA    | 549 | C    |
| 31  | BA    | 550 | A    |
| 31  | BA    | 551 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 31  | BA    | 553 | U    |
| 31  | BA    | 560 | A    |
| 31  | BA    | 561 | C    |
| 31  | BA    | 562 | A    |
| 31  | BA    | 563 | U    |
| 31  | BA    | 570 | A    |
| 31  | BA    | 572 | A    |
| 31  | BA    | 574 | A    |
| 31  | BA    | 576 | U    |
| 31  | BA    | 578 | A    |
| 31  | BA    | 579 | U    |
| 31  | BA    | 584 | A    |
| 31  | BA    | 586 | C    |
| 31  | BA    | 592 | G    |
| 31  | BA    | 595 | C    |
| 31  | BA    | 596 | A    |
| 31  | BA    | 618 | A    |
| 31  | BA    | 624 | A    |
| 31  | BA    | 625 | A    |
| 31  | BA    | 626 | G    |
| 31  | BA    | 631 | A    |
| 31  | BA    | 633 | U    |
| 31  | BA    | 634 | G    |
| 31  | BA    | 640 | A    |
| 31  | BA    | 660 | C    |
| 31  | BA    | 665 | C    |
| 31  | BA    | 673 | C    |
| 31  | BA    | 674 | U    |
| 31  | BA    | 675 | U    |
| 31  | BA    | 683 | U    |
| 31  | BA    | 684 | A    |
| 31  | BA    | 689 | A    |
| 31  | BA    | 694 | A    |
| 31  | BA    | 695 | U    |
| 31  | BA    | 697 | C    |
| 31  | BA    | 704 | U    |
| 31  | BA    | 707 | A    |
| 31  | BA    | 712 | C    |
| 31  | BA    | 713 | A    |
| 31  | BA    | 719 | C    |
| 31  | BA    | 720 | C    |
| 31  | BA    | 721 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 31  | BA    | 722 | A    |
| 31  | BA    | 723 | A    |
| 31  | BA    | 724 | A    |
| 31  | BA    | 725 | C    |
| 31  | BA    | 727 | A    |
| 31  | BA    | 728 | C    |
| 31  | BA    | 744 | A    |
| 31  | BA    | 745 | A    |
| 31  | BA    | 746 | U    |
| 31  | BA    | 747 | U    |
| 31  | BA    | 748 | A    |
| 31  | BA    | 755 | U    |
| 31  | BA    | 763 | C    |
| 31  | BA    | 774 | A    |
| 31  | BA    | 777 | A    |
| 31  | BA    | 778 | A    |
| 31  | BA    | 780 | G    |
| 31  | BA    | 782 | A    |
| 31  | BA    | 783 | A    |
| 31  | BA    | 814 | C    |
| 31  | BA    | 825 | C    |
| 31  | BA    | 843 | C    |
| 31  | BA    | 847 | U    |
| 31  | BA    | 848 | C    |
| 31  | BA    | 850 | A    |
| 31  | BA    | 851 | G    |
| 31  | BA    | 852 | C    |
| 31  | BA    | 853 | A    |
| 31  | BA    | 854 | U    |
| 31  | BA    | 855 | U    |
| 31  | BA    | 859 | A    |
| 31  | BA    | 864 | U    |
| 31  | BA    | 872 | A    |
| 31  | BA    | 889 | C    |
| 31  | BA    | 892 | G    |
| 31  | BA    | 894 | U    |
| 31  | BA    | 895 | U    |
| 31  | BA    | 896 | A    |
| 31  | BA    | 897 | A    |
| 31  | BA    | 900 | G    |
| 31  | BA    | 902 | C    |
| 31  | BA    | 903 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 31  | BA    | 908  | A    |
| 31  | BA    | 909  | U    |
| 31  | BA    | 910  | U    |
| 31  | BA    | 922  | A    |
| 31  | BA    | 924  | G    |
| 31  | BA    | 925  | G    |
| 31  | BA    | 926  | U    |
| 31  | BA    | 931  | U    |
| 31  | BA    | 933  | A    |
| 31  | BA    | 938  | U    |
| 31  | BA    | 947  | A    |
| 31  | BA    | 948  | A    |
| 31  | BA    | 958  | U    |
| 31  | BA    | 959  | G    |
| 31  | BA    | 960  | U    |
| 31  | BA    | 962  | U    |
| 31  | BA    | 964  | A    |
| 31  | BA    | 965  | A    |
| 31  | BA    | 967  | G    |
| 31  | BA    | 969  | C    |
| 31  | BA    | 970  | C    |
| 31  | BA    | 977  | G    |
| 31  | BA    | 983  | U    |
| 31  | BA    | 986  | U    |
| 31  | BA    | 988  | U    |
| 31  | BA    | 992  | U    |
| 31  | BA    | 1008 | A    |
| 31  | BA    | 1015 | C    |
| 31  | BA    | 1016 | C    |
| 31  | BA    | 1018 | U    |
| 31  | BA    | 1026 | A    |
| 31  | BA    | 1027 | G    |
| 31  | BA    | 1028 | A    |
| 31  | BA    | 1038 | A    |
| 31  | BA    | 1041 | A    |
| 31  | BA    | 1045 | U    |
| 31  | BA    | 1050 | C    |
| 31  | BA    | 1051 | G    |
| 31  | BA    | 1055 | A    |
| 31  | BA    | 1056 | G    |
| 31  | BA    | 1057 | A    |
| 31  | BA    | 1063 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 31  | BA    | 1064 | G    |
| 31  | BA    | 1071 | U    |
| 31  | BA    | 1072 | A    |
| 31  | BA    | 1074 | U    |
| 31  | BA    | 1075 | U    |
| 31  | BA    | 1080 | A    |
| 31  | BA    | 1081 | U    |
| 31  | BA    | 1089 | G    |
| 31  | BA    | 1091 | U    |
| 31  | BA    | 1092 | A    |
| 31  | BA    | 1093 | A    |
| 31  | BA    | 1127 | A    |
| 31  | BA    | 1129 | C    |
| 31  | BA    | 1138 | G    |
| 31  | BA    | 1140 | A    |
| 31  | BA    | 1146 | G    |
| 31  | BA    | 1150 | G    |
| 31  | BA    | 1167 | C    |
| 31  | BA    | 1168 | A    |
| 31  | BA    | 1169 | A    |
| 31  | BA    | 1180 | G    |
| 31  | BA    | 1183 | U    |
| 31  | BA    | 1194 | U    |
| 31  | BA    | 1195 | A    |
| 31  | BA    | 1204 | A    |
| 31  | BA    | 1206 | U    |
| 31  | BA    | 1207 | C    |
| 31  | BA    | 1215 | C    |
| 31  | BA    | 1216 | C    |
| 31  | BA    | 1217 | A    |
| 31  | BA    | 1218 | U    |
| 31  | BA    | 1219 | A    |
| 31  | BA    | 1220 | A    |
| 31  | BA    | 1221 | C    |
| 31  | BA    | 1222 | A    |
| 31  | BA    | 1226 | C    |
| 31  | BA    | 1233 | A    |
| 31  | BA    | 1237 | A    |
| 31  | BA    | 1238 | A    |
| 31  | BA    | 1239 | A    |
| 31  | BA    | 1240 | A    |
| 31  | BA    | 1241 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 31  | BA    | 1242 | U    |
| 31  | BA    | 1246 | A    |
| 31  | BA    | 1247 | U    |
| 31  | BA    | 1249 | A    |
| 31  | BA    | 1253 | G    |
| 31  | BA    | 1254 | A    |
| 31  | BA    | 1258 | A    |
| 31  | BA    | 1264 | C    |
| 31  | BA    | 1270 | G    |
| 31  | BA    | 1271 | A    |
| 31  | BA    | 1287 | G    |
| 31  | BA    | 1288 | U    |
| 31  | BA    | 1291 | U    |
| 31  | BA    | 1294 | A    |
| 31  | BA    | 1298 | C    |
| 31  | BA    | 1299 | C    |
| 31  | BA    | 1301 | A    |
| 31  | BA    | 1314 | U    |
| 31  | BA    | 1315 | U    |
| 31  | BA    | 1321 | C    |
| 31  | BA    | 1323 | U    |
| 31  | BA    | 1325 | G    |
| 31  | BA    | 1326 | A    |
| 31  | BA    | 1327 | U    |
| 31  | BA    | 1328 | G    |
| 31  | BA    | 1336 | A    |
| 31  | BA    | 1341 | A    |
| 31  | BA    | 1342 | C    |
| 31  | BA    | 1348 | U    |
| 31  | BA    | 1352 | G    |
| 31  | BA    | 1358 | G    |
| 31  | BA    | 1360 | U    |
| 31  | BA    | 1385 | U    |
| 31  | BA    | 1386 | U    |
| 31  | BA    | 1387 | A    |
| 31  | BA    | 1388 | A    |
| 31  | BA    | 1389 | A    |
| 31  | BA    | 1390 | G    |
| 31  | BA    | 1395 | A    |
| 31  | BA    | 1396 | C    |
| 31  | BA    | 1405 | A    |
| 31  | BA    | 1408 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 31  | BA    | 1420 | A    |
| 31  | BA    | 1421 | A    |
| 31  | BA    | 1425 | A    |
| 31  | BA    | 1426 | G    |
| 31  | BA    | 1429 | C    |
| 31  | BA    | 1432 | U    |
| 31  | BA    | 1433 | U    |
| 31  | BA    | 1436 | U    |
| 31  | BA    | 1438 | U    |
| 31  | BA    | 1445 | U    |
| 31  | BA    | 1448 | A    |
| 31  | BA    | 1453 | U    |
| 31  | BA    | 1455 | C    |
| 31  | BA    | 1457 | A    |
| 31  | BA    | 1465 | A    |
| 31  | BA    | 1468 | A    |
| 31  | BA    | 1474 | G    |
| 31  | BA    | 1493 | A    |
| 31  | BA    | 1494 | A    |
| 31  | BA    | 1498 | C    |
| 31  | BA    | 1504 | A    |
| 31  | BA    | 1505 | G    |
| 31  | BA    | 1509 | U    |
| 31  | BA    | 1514 | A    |
| 31  | BA    | 1521 | U    |
| 31  | BA    | 1526 | U    |
| 31  | BA    | 1527 | U    |
| 31  | BA    | 1528 | A    |
| 31  | BA    | 1531 | C    |
| 31  | BA    | 1532 | U    |
| 31  | BA    | 1533 | A    |
| 31  | BA    | 1536 | U    |
| 31  | BA    | 1548 | A    |
| 31  | BA    | 1551 | C    |
| 31  | BA    | 1552 | C    |
| 31  | BA    | 1553 | A    |
| 31  | BA    | 1554 | G    |
| 31  | BA    | 1558 | U    |
| 31  | BA    | 1559 | A    |
| 31  | BA    | 1569 | A    |
| 31  | BA    | 1571 | A    |
| 74  | BB    | 3    | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 74  | BB    | 4   | A    |
| 74  | BB    | 5   | A    |
| 74  | BB    | 7   | G    |
| 74  | BB    | 8   | U    |
| 74  | BB    | 9   | A    |
| 74  | BB    | 13  | U    |
| 74  | BB    | 21  | C    |
| 74  | BB    | 23  | A    |
| 74  | BB    | 29  | G    |
| 74  | BB    | 34  | U    |
| 74  | BB    | 43  | C    |
| 74  | BB    | 44  | U    |
| 74  | BB    | 46  | G    |
| 74  | BB    | 47  | A    |
| 74  | BB    | 48  | U    |
| 74  | BB    | 69  | C    |
| 74  | BB    | 70  | A    |

All (4) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 31  | AA    | 530 | G    |
| 31  | AA    | 825 | C    |
| 46  | AY    | 44  | U    |
| 31  | BA    | 48  | U    |

## 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 338 ligands modelled in this entry, 331 are monoatomic - leaving 7 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 |
| 91  | FME  | AV    | 101   | 46   | 8,9,10       | 0.96 | 0        | 7,9,11      | 0.89 | 0        |
| 93  | 5GP  | BA    | 15901 | 88   | 26,26,26     | 1.00 | 2 (7%)   | 40,40,40    | 1.67 | 7 (17%)  |
| 90  | SPM  | BA    | 15903 | -    | 13,13,13     | 0.34 | 0        | 12,12,12    | 0.78 | 0        |
| 92  | GTP  | Ag    | 500   | 88   | 30,34,34     | 0.83 | 1 (3%)   | 46,54,54    | 1.83 | 11 (23%) |
| 94  | GNP  | BC    | 802   | 88   | 33,34,34     | 1.29 | 5 (15%)  | 46,54,54    | 0.76 | 2 (4%)   |
| 90  | SPM  | BA    | 15902 | -    | 13,13,13     | 0.34 | 0        | 12,12,12    | 0.76 | 0        |
| 90  | SPM  | AA    | 16801 | -    | 13,13,13     | 0.33 | 0        | 12,12,12    | 0.80 | 0        |

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

| Mol | Type | Chain | Res   | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-------|------|---------|------------|---------|
| 91  | FME  | AV    | 101   | 46   | -       | 3/7/9/11   | -       |
| 93  | 5GP  | BA    | 15901 | 88   | -       | 0/10/26/26 | 0/3/3/3 |
| 90  | SPM  | BA    | 15903 | -    | -       | 1/11/11/11 | -       |
| 92  | GTP  | Ag    | 500   | 88   | -       | 1/22/38/38 | 0/3/3/3 |
| 94  | GNP  | BC    | 802   | 88   | -       | 9/18/38/38 | 0/3/3/3 |
| 90  | SPM  | BA    | 15902 | -    | -       | 1/11/11/11 | -       |
| 90  | SPM  | AA    | 16801 | -    | -       | 2/11/11/11 | -       |

All (8) bond length outliers are listed below:

| Mol | Chain | Res   | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-------|------|--------|-------|-------------|----------|
| 94  | BC    | 802   | GNP  | PB-O3A | 4.53  | 1.64        | 1.59     |
| 94  | BC    | 802   | GNP  | PB-O1B | 3.05  | 1.51        | 1.46     |
| 94  | BC    | 802   | GNP  | PG-N3B | 2.98  | 1.71        | 1.63     |
| 93  | BA    | 15901 | 5GP  | C6-N1  | -2.58 | 1.34        | 1.38     |
| 94  | BC    | 802   | GNP  | PG-O1G | 2.53  | 1.50        | 1.46     |
| 92  | Ag    | 500   | GTP  | C2-N3  | 2.25  | 1.38        | 1.33     |
| 94  | BC    | 802   | GNP  | PB-O2B | -2.15 | 1.51        | 1.56     |
| 93  | BA    | 15901 | 5GP  | C5-N7  | -2.08 | 1.35        | 1.39     |

All (20) bond angle outliers are listed below:

| Mol | Chain | Res   | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|-------|------|-------------|-------|-------------|----------|
| 93  | BA    | 15901 | 5GP  | C5-C4-N3    | -5.60 | 119.37      | 128.46   |
| 92  | Ag    | 500   | GTP  | C5-C4-N3    | -5.39 | 119.72      | 128.46   |
| 92  | Ag    | 500   | GTP  | C2-N3-C4    | 4.70  | 120.67      | 112.30   |
| 93  | BA    | 15901 | 5GP  | C2-N3-C4    | 4.31  | 119.98      | 112.30   |
| 92  | Ag    | 500   | GTP  | PA-O3A-PB   | -3.91 | 119.41      | 132.83   |
| 92  | Ag    | 500   | GTP  | PB-O3B-PG   | -3.83 | 119.67      | 132.83   |
| 92  | Ag    | 500   | GTP  | N9-C4-N3    | 3.54  | 133.05      | 125.94   |
| 93  | BA    | 15901 | 5GP  | N9-C4-N3    | 3.54  | 133.04      | 125.94   |
| 92  | Ag    | 500   | GTP  | C2-N1-C6    | -3.02 | 119.59      | 125.10   |
| 92  | Ag    | 500   | GTP  | C5-C6-N1    | 2.58  | 119.73      | 113.19   |
| 92  | Ag    | 500   | GTP  | C8-N7-C5    | 2.57  | 108.90      | 104.24   |
| 94  | BC    | 802   | GNP  | PB-O3A-PA   | -2.54 | 123.67      | 132.62   |
| 92  | Ag    | 500   | GTP  | N9-C8-N7    | -2.52 | 108.64      | 113.39   |
| 93  | BA    | 15901 | 5GP  | C5-C6-N1    | 2.47  | 119.45      | 113.19   |
| 93  | BA    | 15901 | 5GP  | O6-C6-C5    | -2.44 | 120.14      | 126.60   |
| 92  | Ag    | 500   | GTP  | O6-C6-C5    | -2.39 | 120.25      | 126.60   |
| 92  | Ag    | 500   | GTP  | C3'-C2'-C1' | 2.36  | 105.91      | 101.43   |
| 93  | BA    | 15901 | 5GP  | C2-N1-C6    | -2.28 | 120.93      | 125.10   |
| 93  | BA    | 15901 | 5GP  | N9-C8-N7    | -2.24 | 109.18      | 113.39   |
| 94  | BC    | 802   | GNP  | O1B-PB-N3B  | -2.17 | 108.57      | 111.77   |

There are no chirality outliers.

All (17) torsion outliers are listed below:

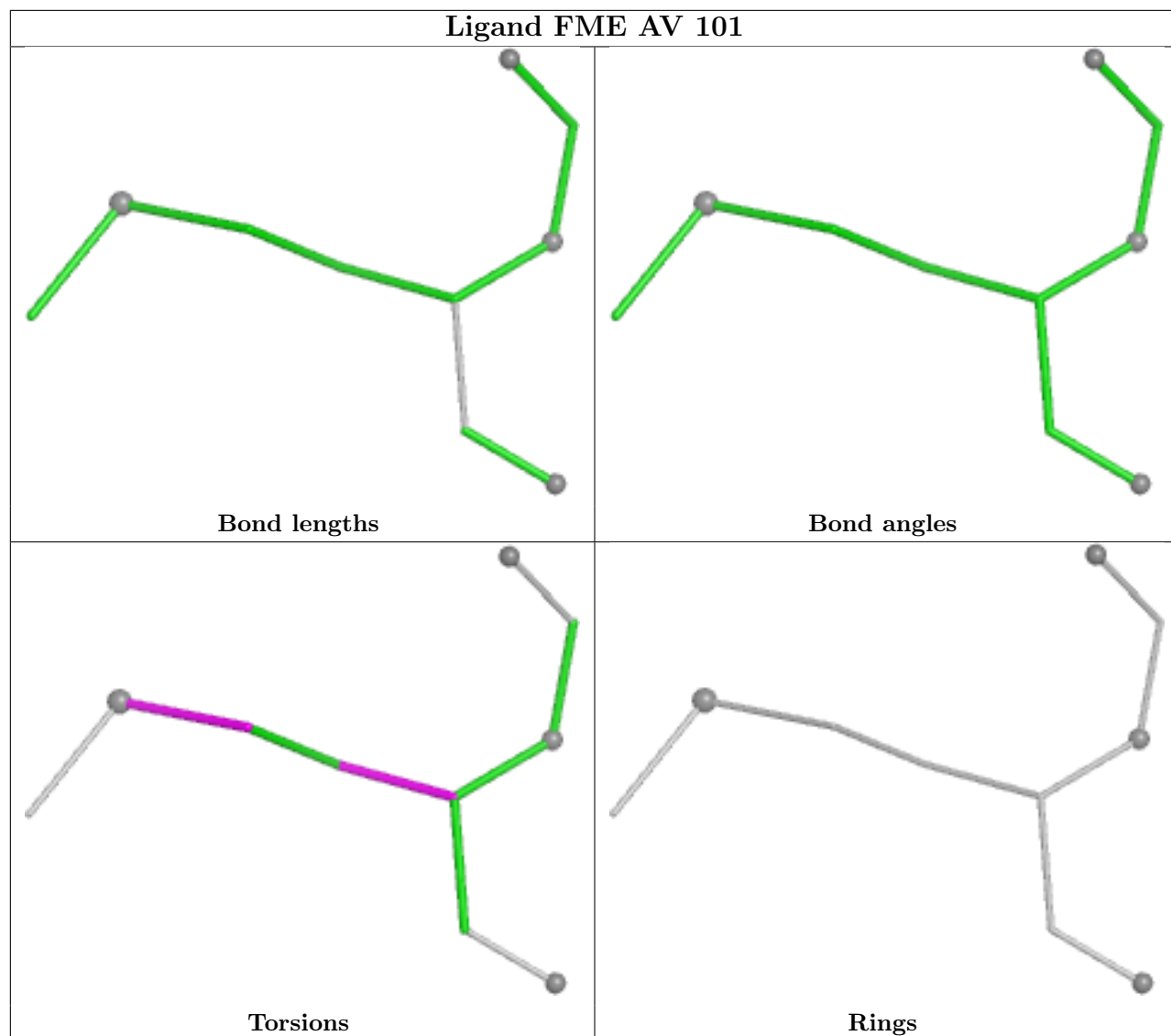
| Mol | Chain | Res   | Type | Atoms           |
|-----|-------|-------|------|-----------------|
| 91  | AV    | 101   | FME  | N-CA-CB-CG      |
| 94  | BC    | 802   | GNP  | PB-N3B-PG-O1G   |
| 94  | BC    | 802   | GNP  | PG-N3B-PB-O1B   |
| 94  | BC    | 802   | GNP  | PA-O3A-PB-O1B   |
| 94  | BC    | 802   | GNP  | PA-O3A-PB-O2B   |
| 94  | BC    | 802   | GNP  | C5'-O5'-PA-O3A  |
| 94  | BC    | 802   | GNP  | C5'-O5'-PA-O2A  |
| 94  | BC    | 802   | GNP  | O4'-C4'-C5'-O5' |
| 90  | BA    | 15903 | SPM  | N5-C6-C7-C8     |
| 90  | AA    | 16801 | SPM  | C8-C9-N10-C11   |
| 94  | BC    | 802   | GNP  | C3'-C4'-C5'-O5' |
| 91  | AV    | 101   | FME  | CB-CG-SD-CE     |
| 94  | BC    | 802   | GNP  | C5'-O5'-PA-O1A  |
| 91  | AV    | 101   | FME  | C-CA-CB-CG      |
| 92  | Ag    | 500   | GTP  | C4'-C5'-O5'-PA  |
| 90  | AA    | 16801 | SPM  | C7-C6-N5-C4     |
| 90  | BA    | 15902 | SPM  | C8-C9-N10-C11   |

There are no ring outliers.

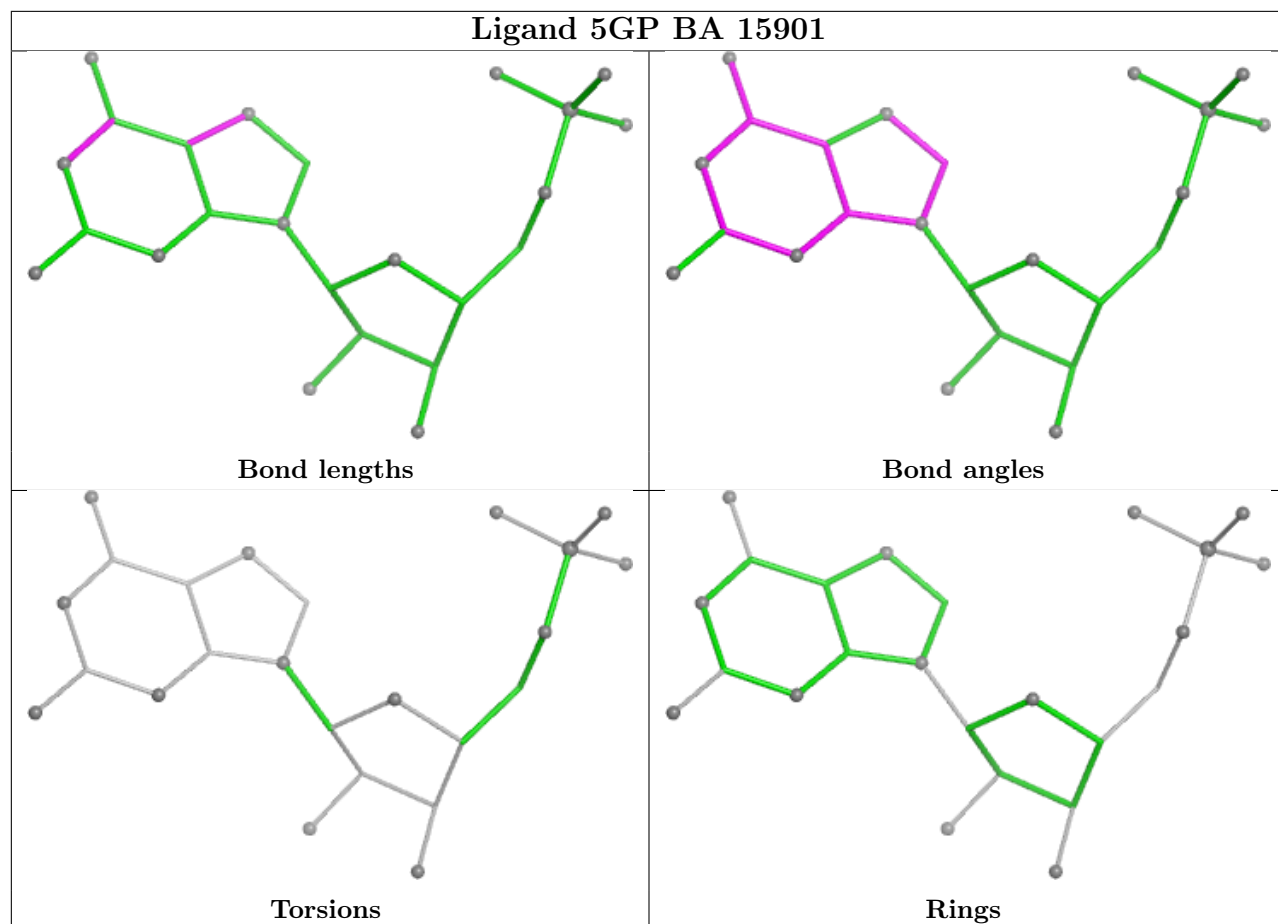
1 monomer is involved in 3 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 94  | BC    | 802 | GNP  | 3       | 0            |

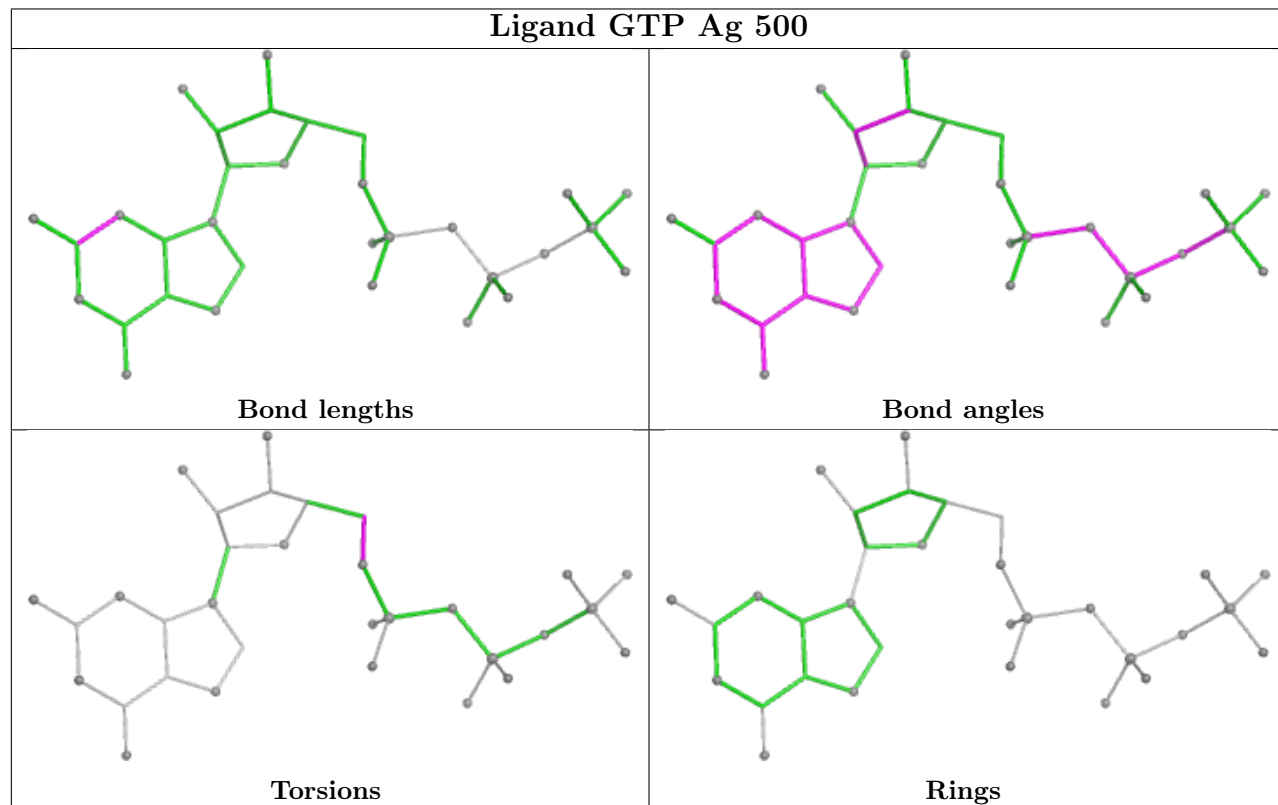
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

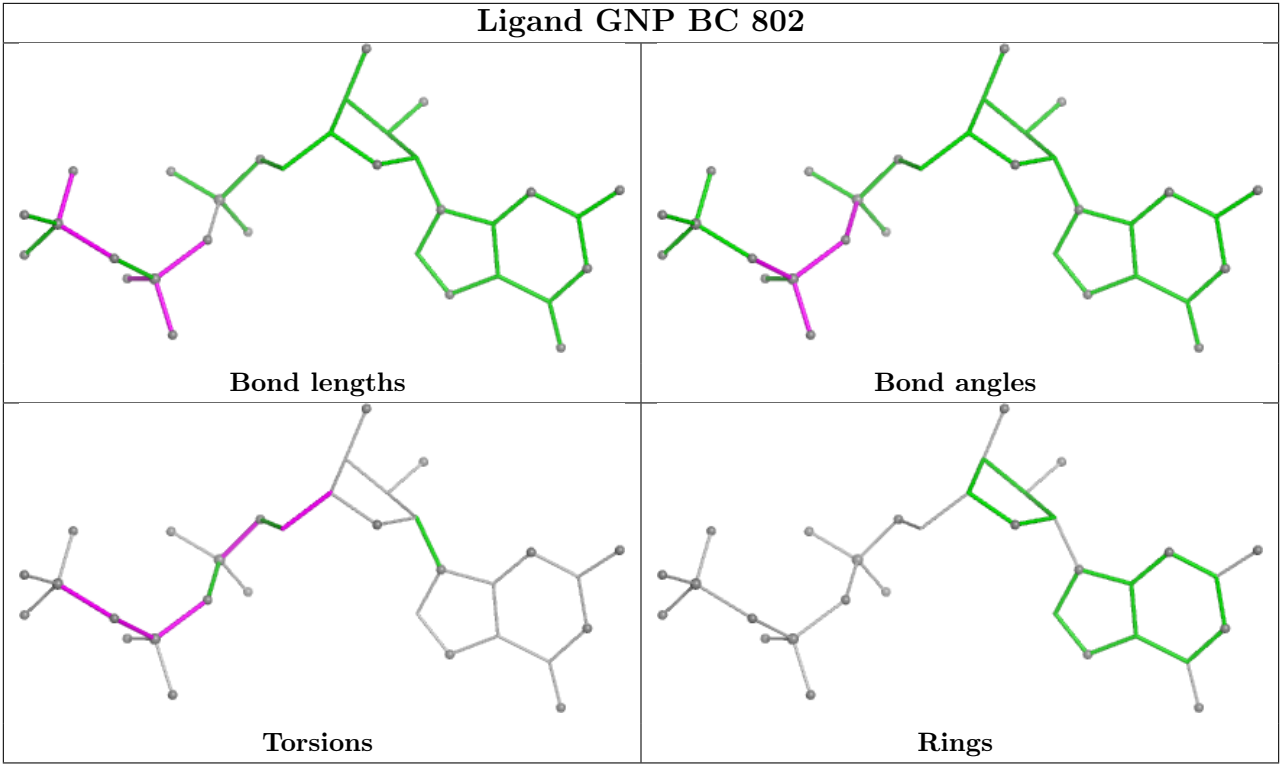


## Ligand 5GP BA 15901



## Ligand GTP Ag 500





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 |
|-----|-------|------------------|
| 63  | Ao    | 1                |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | Ao    | 234:VAL   | C      | 240:THR   | N      | 8.13         |

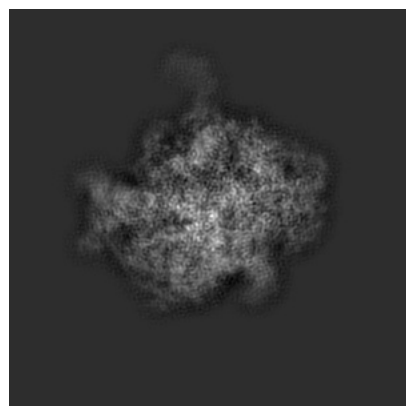
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10779. These allow visual inspection of the internal detail of the map and identification of artifacts.

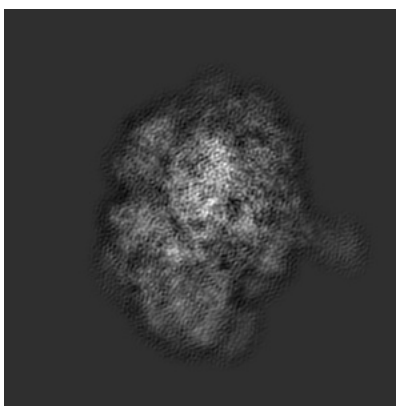
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

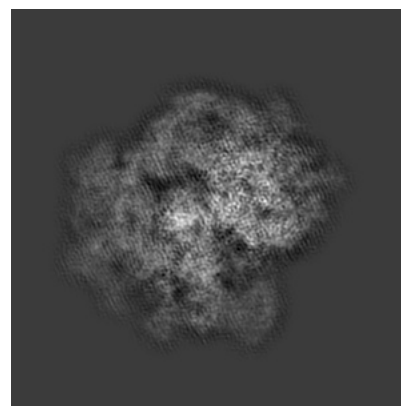
#### 6.1.1 Primary map



X

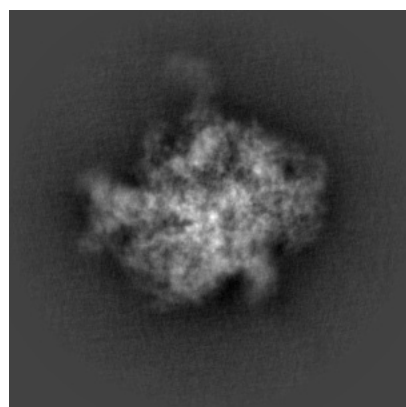


Y

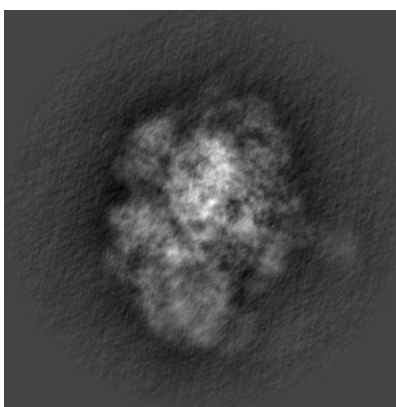


Z

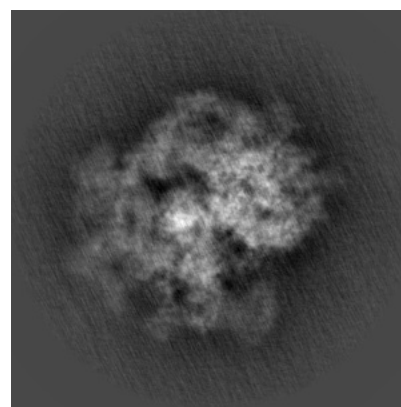
#### 6.1.2 Raw map



X



Y

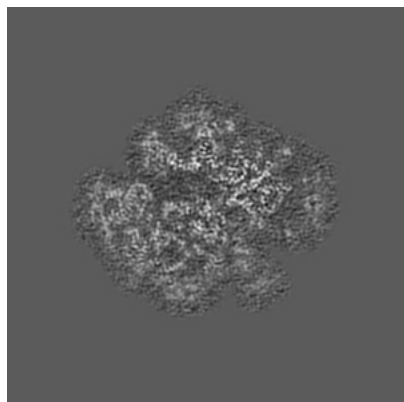


Z

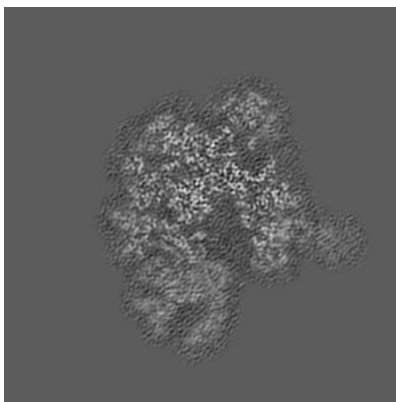
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

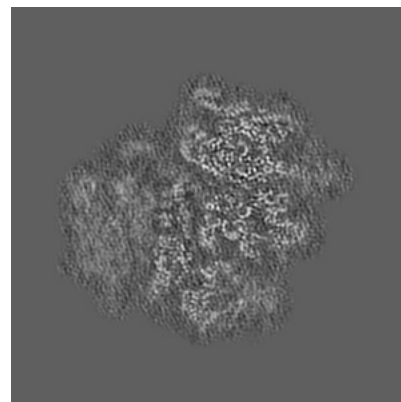
### 6.2.1 Primary map



X Index: 160

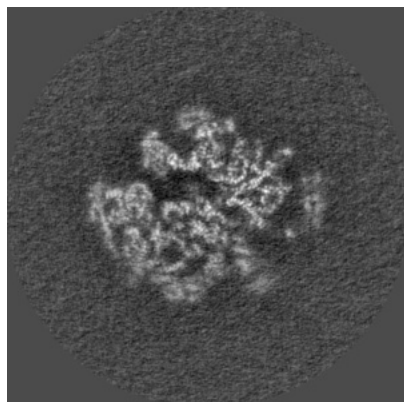


Y Index: 160

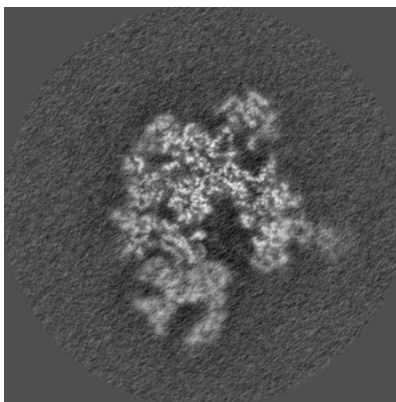


Z Index: 160

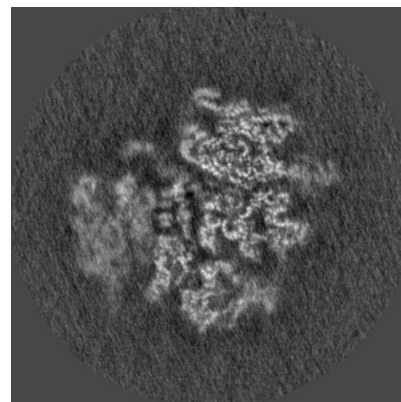
### 6.2.2 Raw map



X Index: 160



Y Index: 160

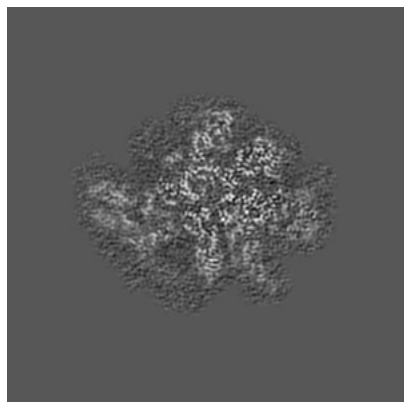


Z Index: 160

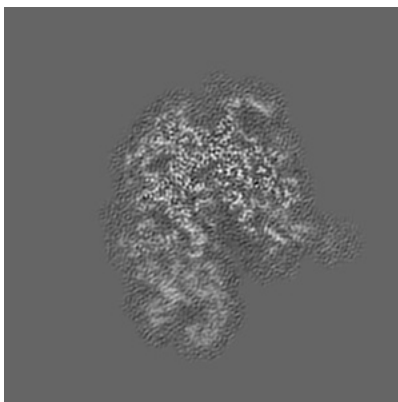
The images above show central slices of the map in three orthogonal directions.

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

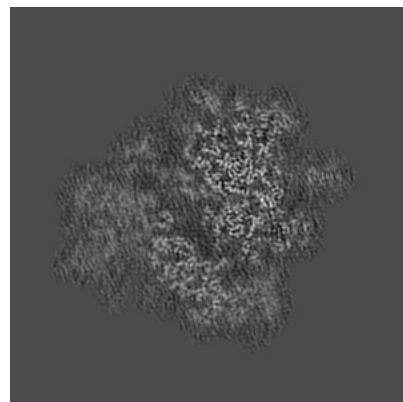
### 6.3.1 Primary map



X Index: 168

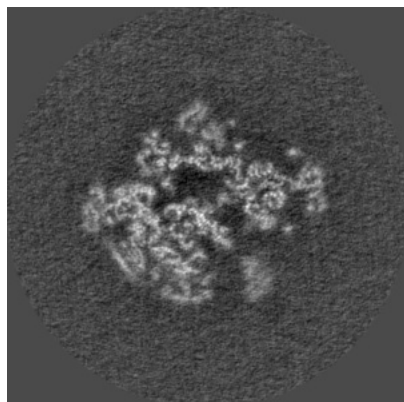


Y Index: 166

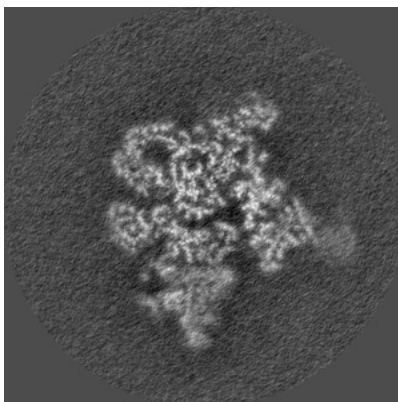


Z Index: 166

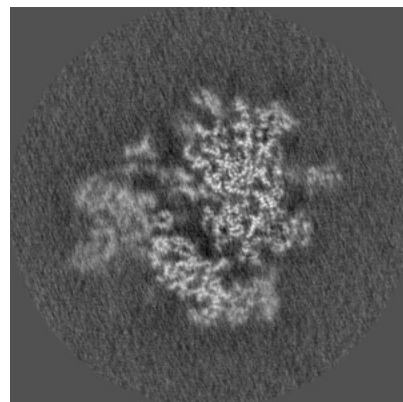
### 6.3.2 Raw map



X Index: 154



Y Index: 150

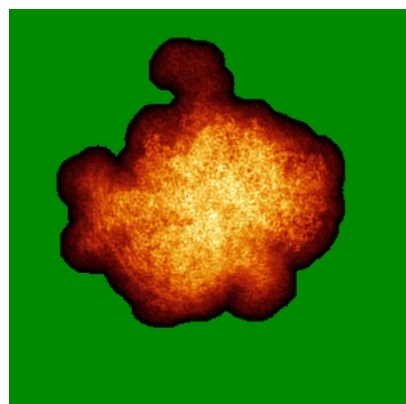


Z Index: 166

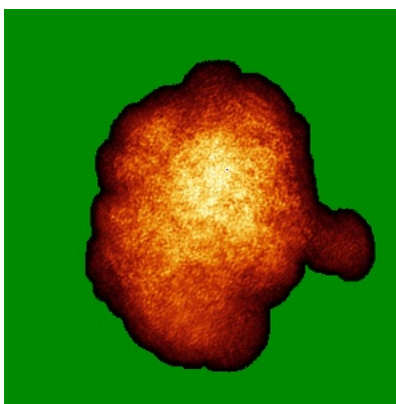
The images above show the largest variance slices of the map in three orthogonal directions.

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

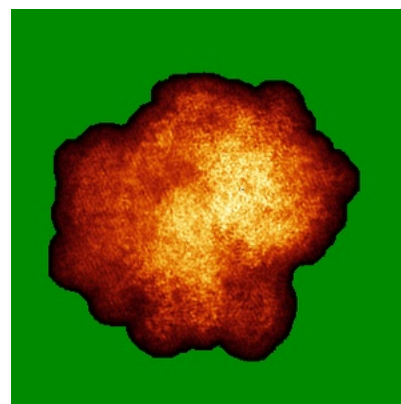
### 6.4.1 Primary map



X

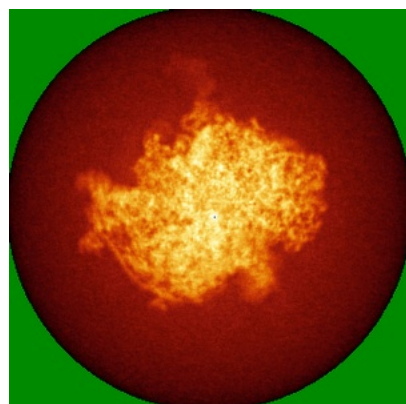


Y

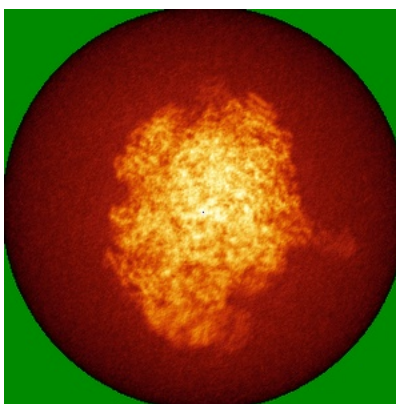


Z

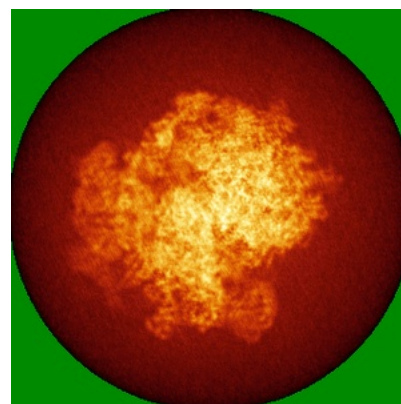
### 6.4.2 Raw map



X



Y

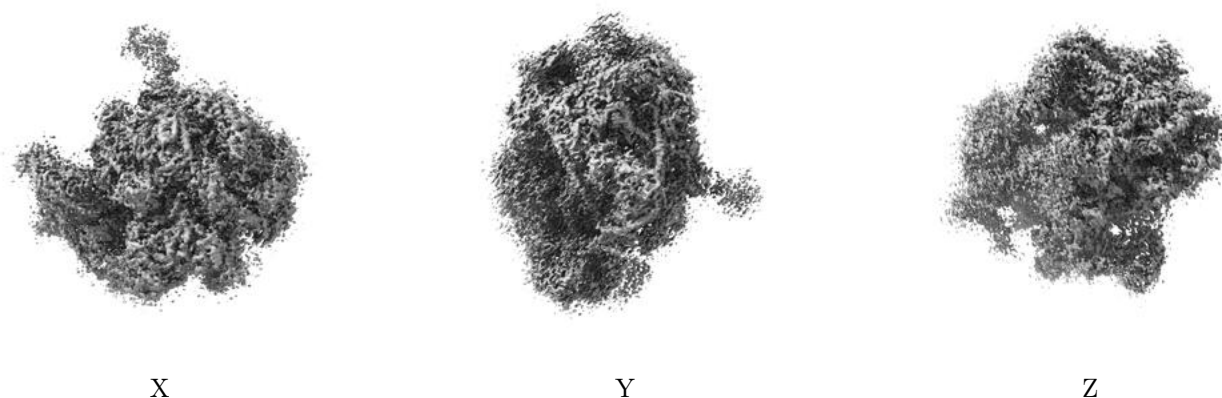


Z

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

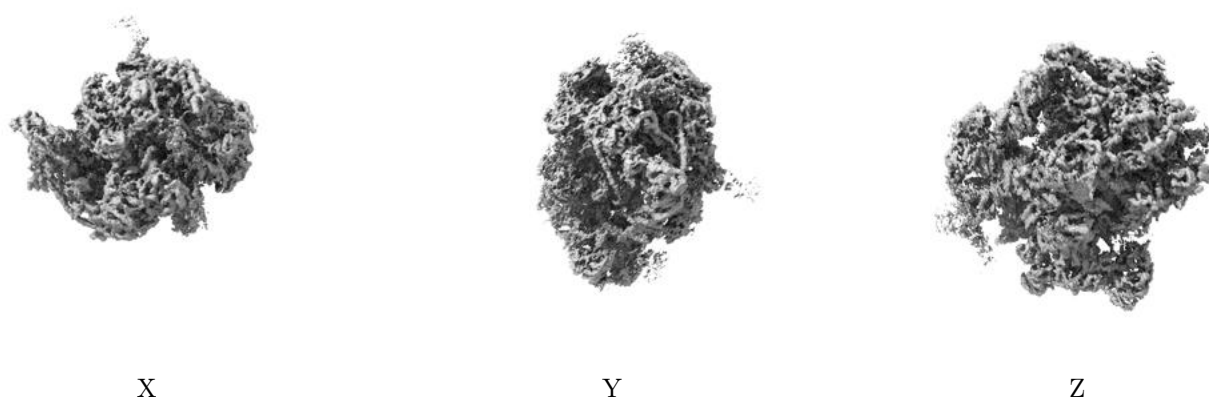
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.045. 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.

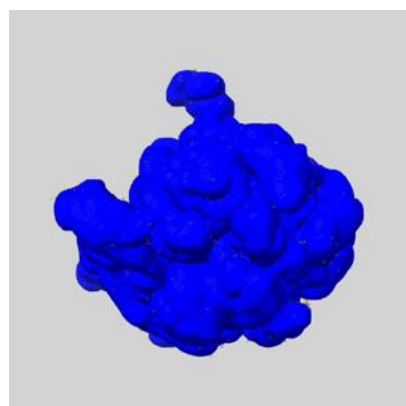
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

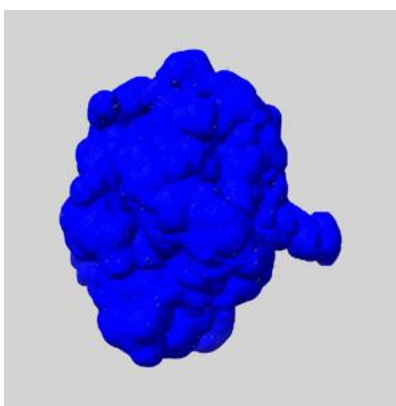
A mask typically either:

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

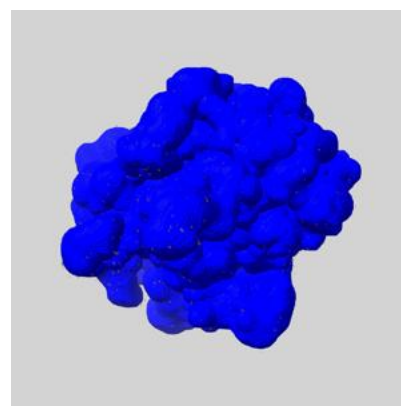
### 6.6.1 emd\_10779\_msk\_1.map [i](#)



X



Y

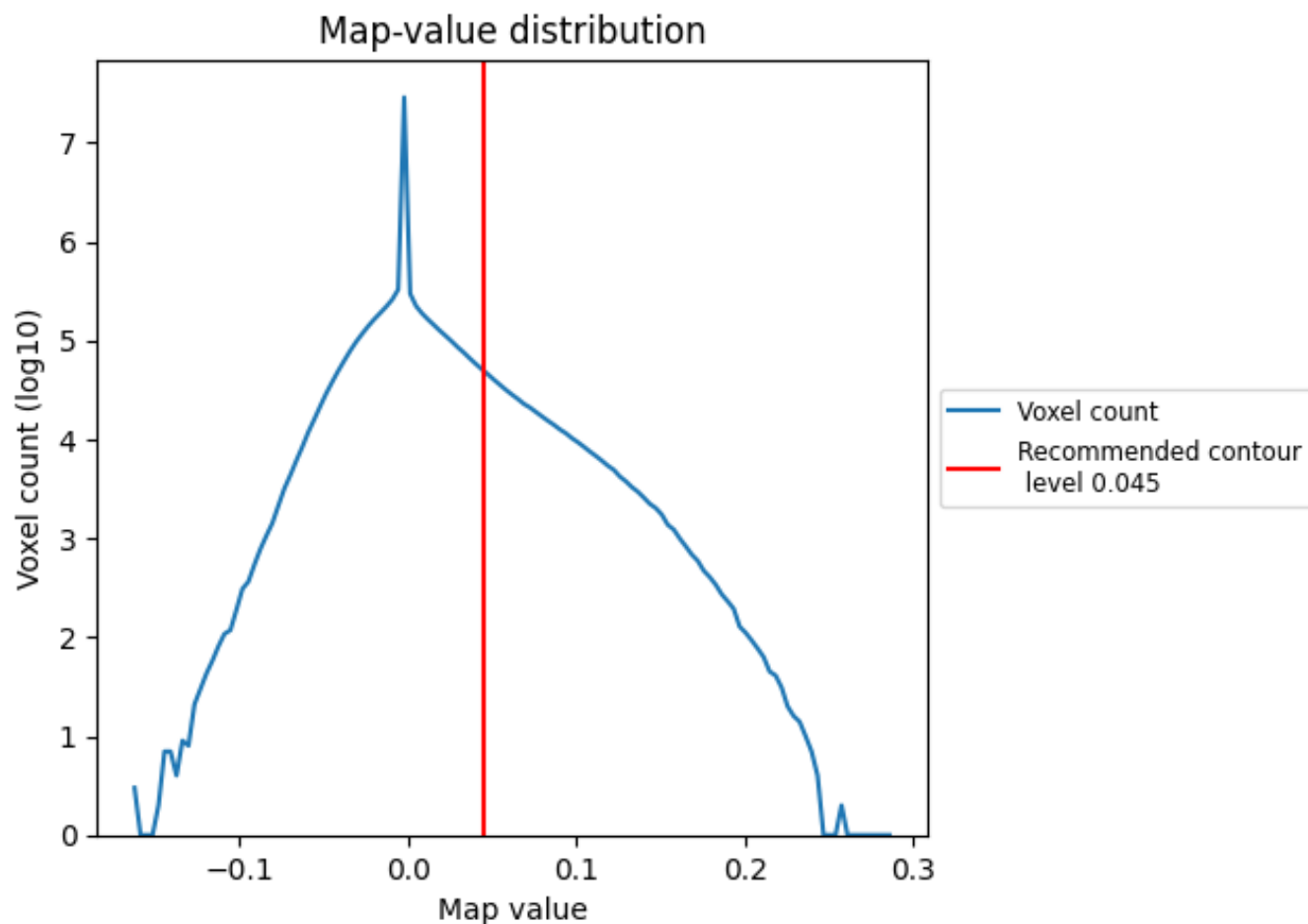


Z

## 7 Map analysis [i](#)

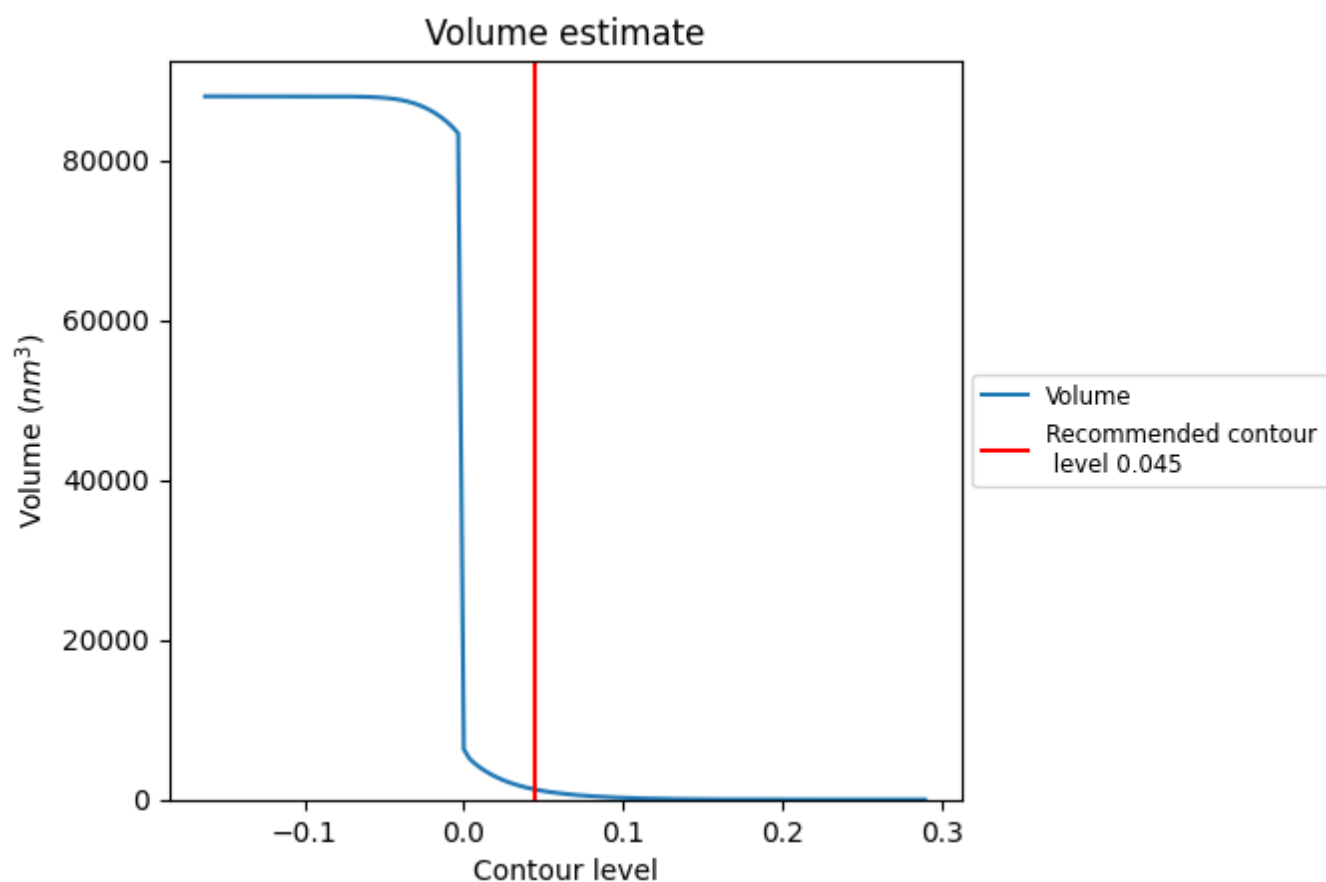
This section contains the results of statistical analysis of the map.

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



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

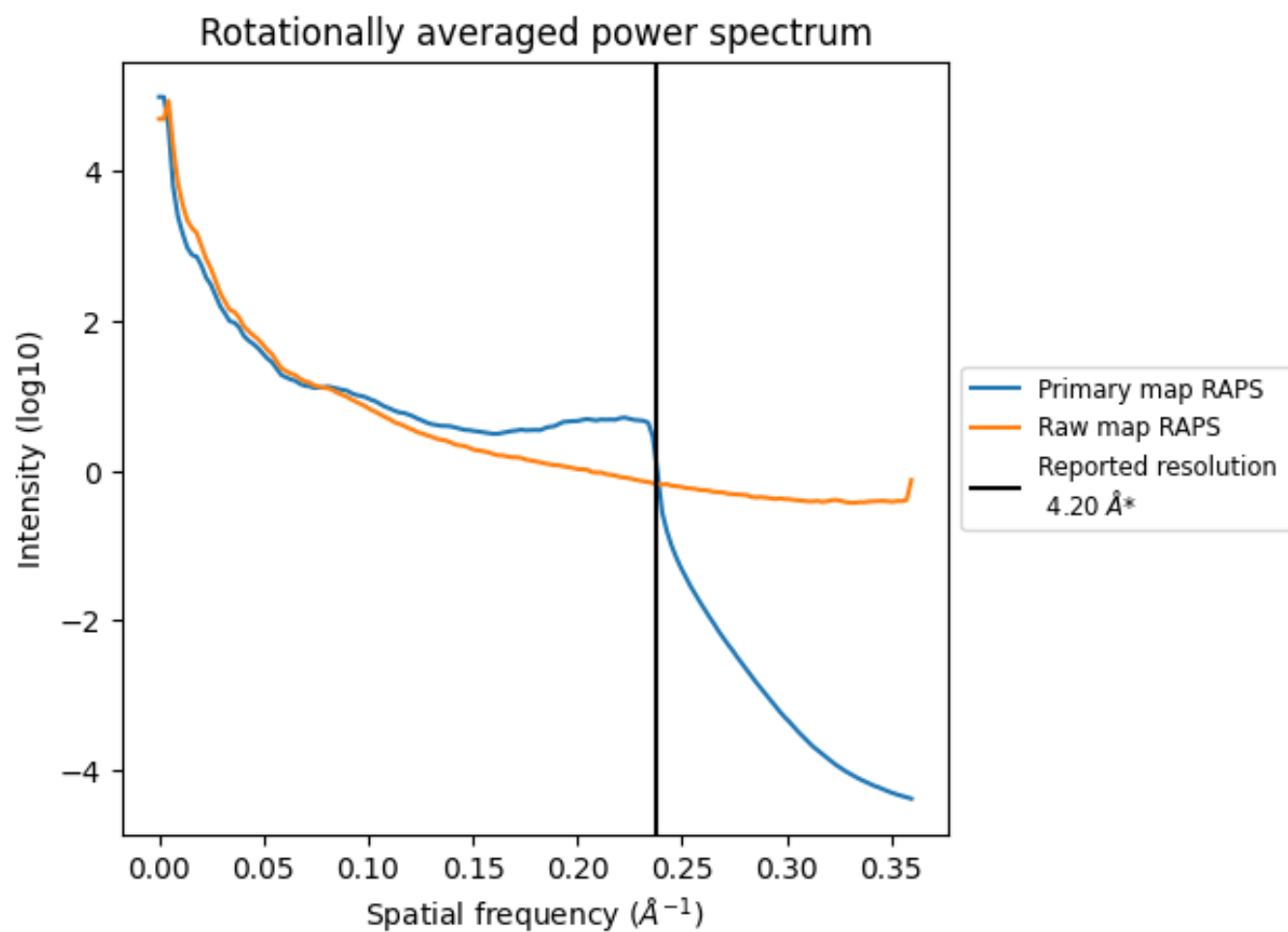
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1253 nm<sup>3</sup>; this corresponds to an approximate mass of 1132 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 ⓘ

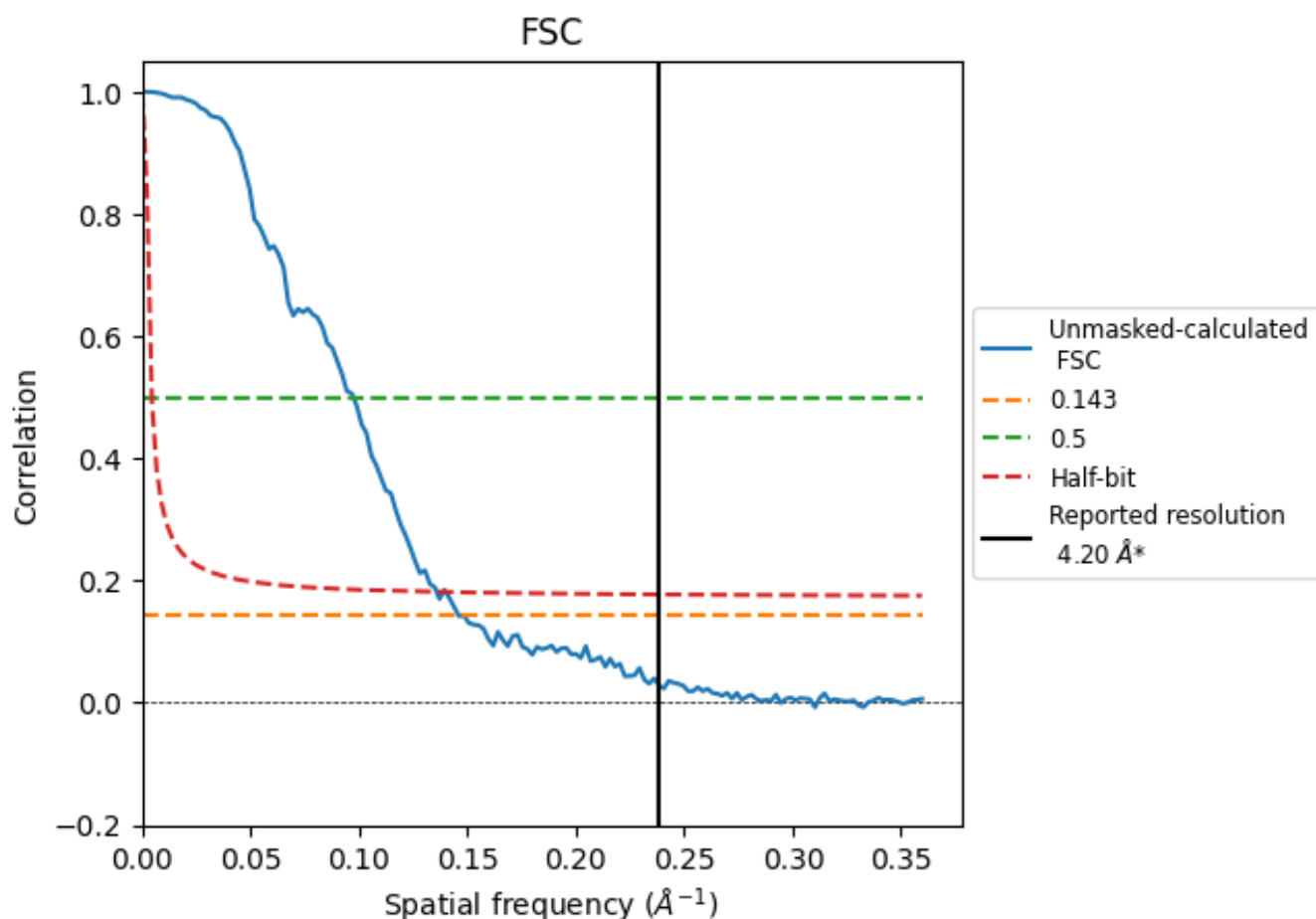


\*Reported resolution corresponds to spatial frequency of 0.238 Å<sup>-1</sup>

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

## 8.2 Resolution estimates [i](#)

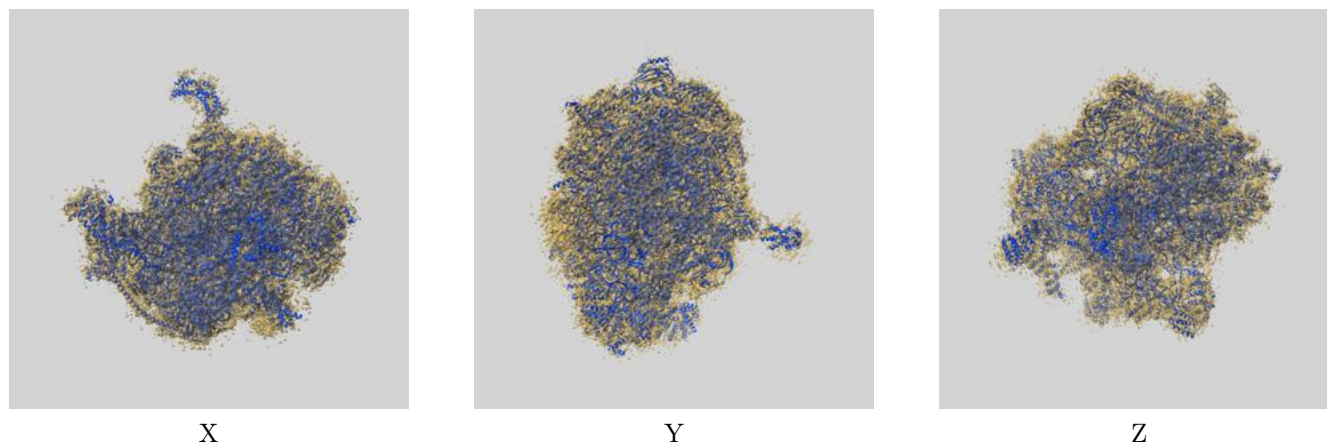
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |       |          |
|---------------------------|------------------------------------|-------|----------|
|                           | 0.143                              | 0.5   | Half-bit |
| Reported by author        | 4.20                               | -     | -        |
| Author-provided FSC curve | -                                  | -     | -        |
| Unmasked-calculated*      | 6.85                               | 10.27 | 7.36     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.85 differs from the reported value 4.2 by more than 10 %

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

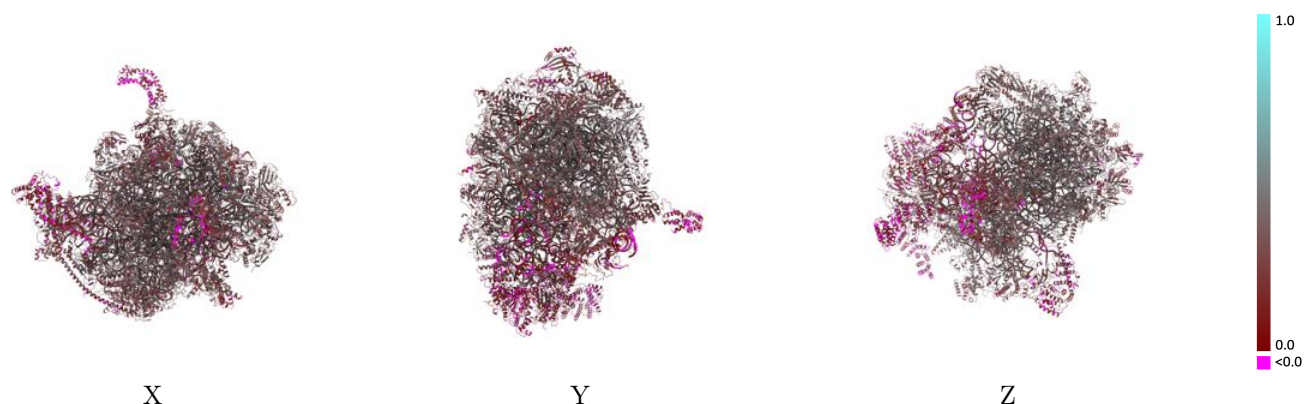
This section contains information regarding the fit between EMDB map EMD-10779 and PDB model 6YDW. Per-residue inclusion information can be found in section [3](#) on page [26](#).

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



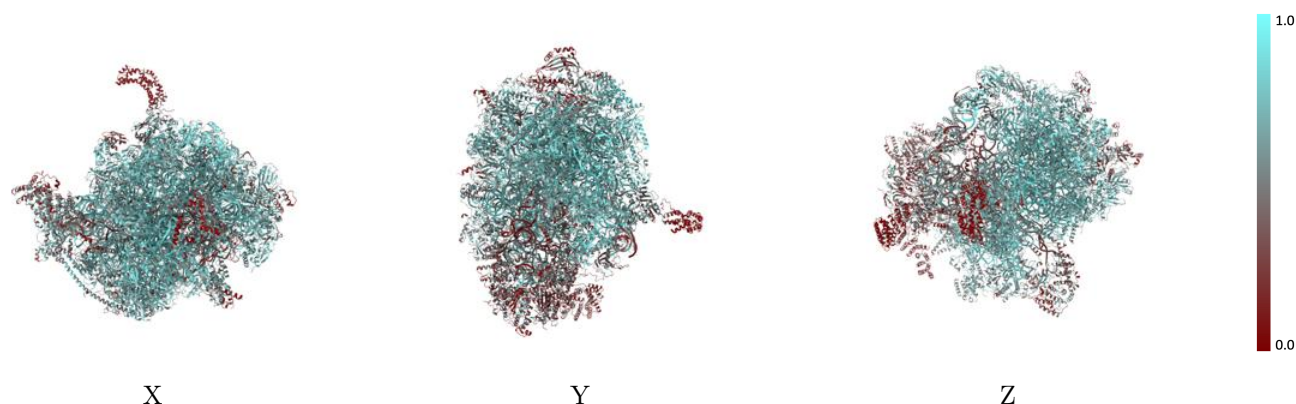
The images above show the 3D surface view of the map at the recommended contour level 0.045 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



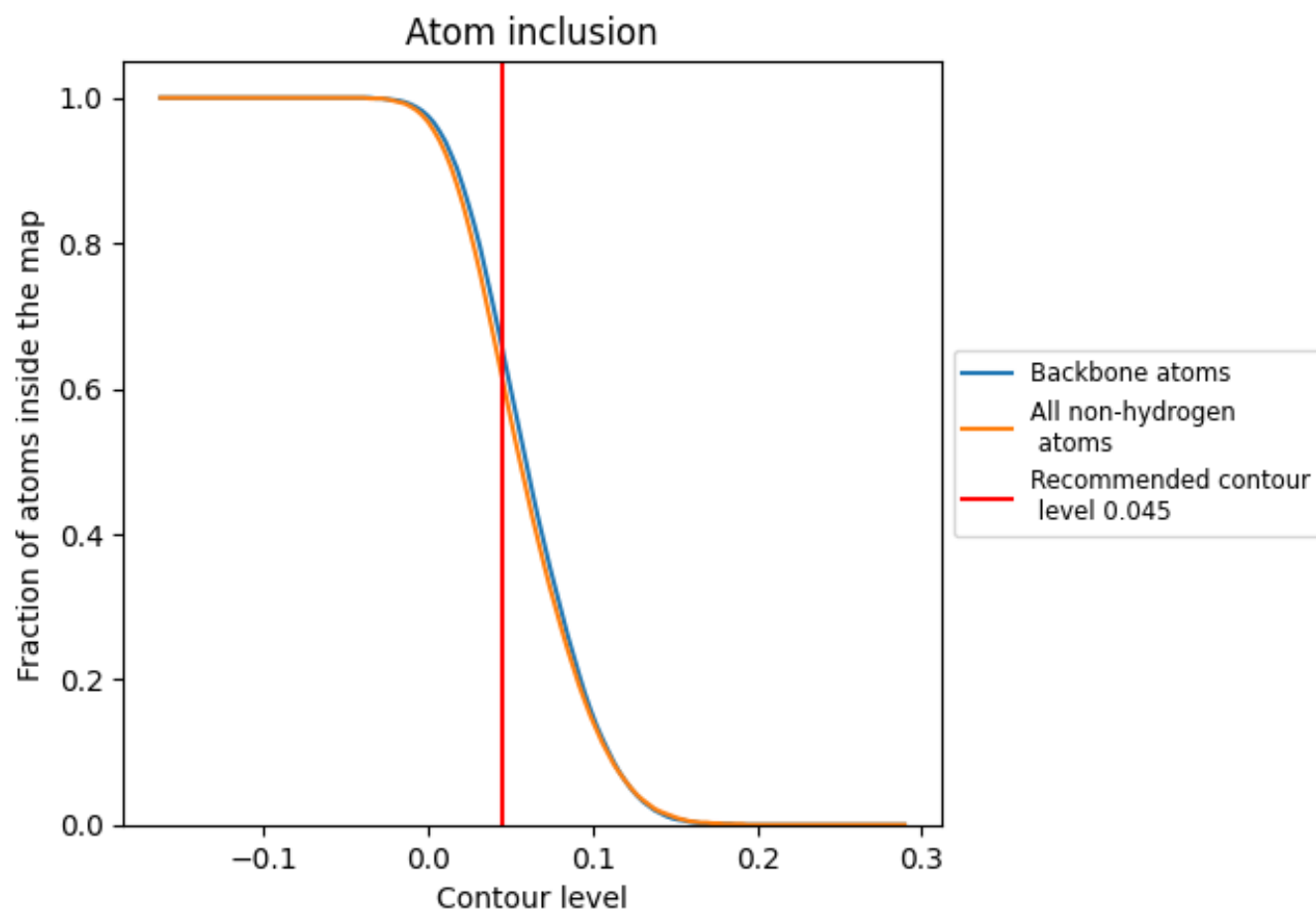
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.045).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 66% of all backbone atoms, 62% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.045) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.6160   |  0.3100   |
| AA    |  0.7160   |  0.3050   |
| AB    |  0.6280   |  0.3230   |
| AC    |  0.3190   |  0.2000   |
| AE    |  0.4730   |  0.3040   |
| AF    |  0.5390   |  0.2990   |
| AG    |  0.3430   |  0.1640   |
| AI    |  0.4420   |  0.2460   |
| AJ    |  0.3430   |  0.2150   |
| AK    |  0.5650   |  0.3020   |
| AL    |  0.6430   |  0.4010   |
| AN    |  0.3930   |  0.2180   |
| AO    |  0.5290   |  0.2940   |
| AP    |  0.6470   |  0.3250   |
| AQ    |  0.6330  |  0.3610  |
| AR    |  0.5980 |  0.3150 |
| AU    |  0.6260 |  0.3520 |
| AV    |  0.6020 |  0.2450 |
| AX    |  0.6670 |  0.3200 |
| AY    |  0.2070 |  0.1010 |
| AZ    |  0.3890 |  0.1530 |
| Aa    |  0.5870 |  0.2900 |
| Ab    |  0.5550 |  0.2810 |
| Ac    |  0.6280 |  0.3450 |
| Ad    |  0.5920 |  0.2550 |
| Ae    |  0.3390 |  0.1420 |
| Af    |  0.5850 |  0.3250 |
| Ag    |  0.3160 |  0.1270 |
| Ah    |  0.2600 |  0.1710 |
| Ai    |  0.3430 |  0.2060 |
| Aj    |  0.4880 |  0.2530 |
| Ak    |  0.3240 |  0.1790 |
| Am    |  0.3950 |  0.2510 |
| An    |  0.5870 |  0.3470 |
| Ao    |  0.1450 |  0.0880 |



*Continued on next page...*

*Continued from previous page...*

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| Ap    |  0.6180   |  0.3150   |
| B0    |  0.7330   |  0.4150   |
| B1    |  0.5970   |  0.3470   |
| B2    |  0.6690   |  0.3460   |
| B3    |  0.7250   |  0.4110   |
| B4    |  0.4970   |  0.2140   |
| B5    |  0.6870   |  0.3720   |
| B6    |  0.4520   |  0.2850   |
| B7    |  0.7320   |  0.4100   |
| B8    |  0.6960   |  0.4170   |
| B9    |  0.7540   |  0.4190   |
| BA    |  0.8230   |  0.3750   |
| BB    |  0.6390   |  0.2140   |
| BC    |  0.6490   |  0.3510   |
| BD    |  0.6960   |  0.3900   |
| BE    |  0.7110   |  0.3890   |
| BF    |  0.6830   |  0.3830   |
| BI    |  0.5330  |  0.3160  |
| BJ    |  0.4620 |  0.2430 |
| BK    |  0.5950 |  0.2900 |
| BN    |  0.7450 |  0.4160 |
| BO    |  0.6410 |  0.4040 |
| BP    |  0.7030 |  0.3790 |
| BQ    |  0.7110 |  0.3970 |
| BR    |  0.7110 |  0.3900 |
| BS    |  0.6980 |  0.3500 |
| BT    |  0.6730 |  0.3730 |
| BU    |  0.7170 |  0.3910 |
| BV    |  0.7320 |  0.4080 |
| BW    |  0.7010 |  0.4040 |
| BX    |  0.6290 |  0.3680 |
| BY    |  0.3630 |  0.2760 |
| Ba    |  0.6840 |  0.3490 |
| Bb    |  0.6930 |  0.3390 |
| Bc    |  0.6640 |  0.3290 |
| Bd    |  0.4510 |  0.1900 |
| Be    |  0.5560 |  0.3240 |
| Bf    |  0.6740 |  0.3510 |
| Bg    |  0.7130 |  0.4040 |
| Bh    |  0.6940 |  0.3450 |
| Bi    |  0.2990 |  0.2280 |
| Bj    |  0.4430 |  0.1670 |

*Continued on next page...*

*Continued from previous page...*

| Chain | Atom inclusion                                                                            | Q-score                                                                                   |
|-------|-------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------|
| Bk    |  0.4650  |  0.2380  |
| Bl    |  0.7350  |  0.3890  |
| Bm    |  0.3850  |  0.2860  |
| Bn    |  0.6920  |  0.3910  |
| Bo    |  0.7190  |  0.3680  |
| Bp    |  0.5250  |  0.2570  |
| Bq    |  0.6270  |  0.2870  |
| Bt    |  0.7330  |  0.3940  |
| Bu    |  0.5090  |  0.2650  |
| Bv    |  0.5630  |  0.2700  |
| Bw    |  0.6790  |  0.3480  |
| Bx    |  0.6960  |  0.3650  |
| CL    |  0.0890  |  0.0840  |
| DL    |  0.1740  |  0.1540  |
| EL    |  0.0810  |  0.0630  |
| FL    |  0.0850  |  0.0830  |
| GL    |  0.0470  |  0.0660  |
| HL    |  0.0490  |  0.1430  |
| LL    |  0.2000 |  0.1800 |