



## Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 10:05 AM UTC

PDB ID : 6XU7 / pdb\_00006xu7  
EMDB ID : EMD-10623  
Title : Drosophila melanogaster Testis polysome ribosome  
Authors : Hopes, T.; Agapiou, M.; Norris, K.; McCarthy, C.G.P.; OConnell, M.J.;  
Fontana, J.; Aspden, J.L.  
Deposited on : 2020-01-17  
Resolution : 4.90 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:

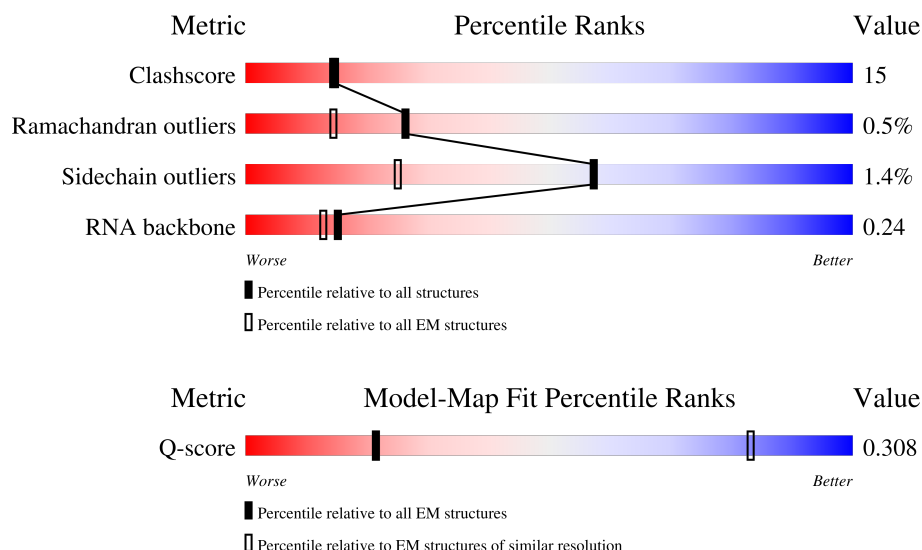
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins)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

# 1 Overall quality at a glance

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

The reported resolution of this entry is 4.90 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.



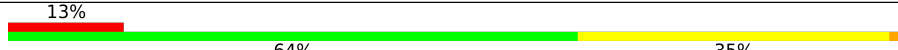
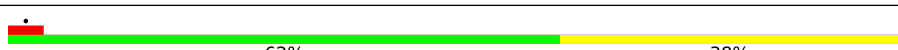
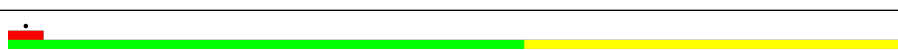
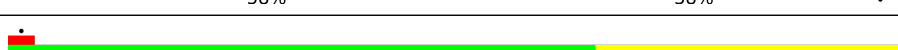
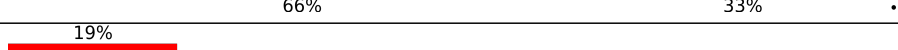
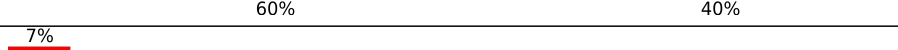
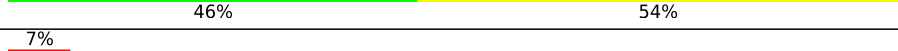
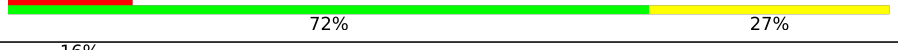
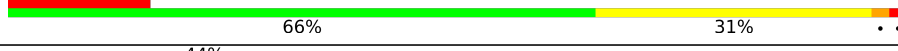
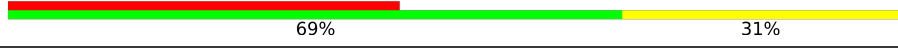
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| RNA backbone          | 8273                        | 3508                        | -                                                        |
| Q-score               | -                           | 25397                       | 1274 ( 4.40 - 5.40 )                                     |

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   | AA    | 218    |                  |
| 2   | CA    | 253    |                  |
| 3   | AB    | 220    |                  |

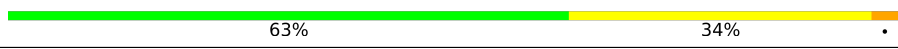
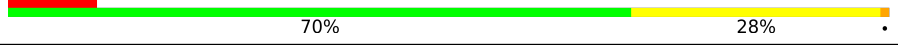
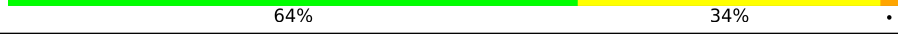
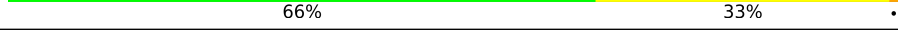
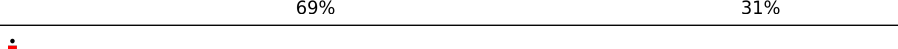
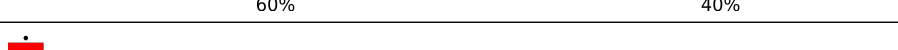
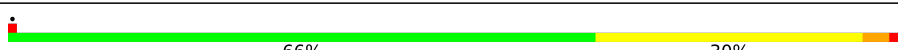
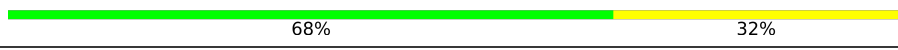
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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 4   | CB    | 414    |    |
| 5   | AC    | 227    |    |
| 6   | CC    | 392    |    |
| 7   | Ag    | 318    |    |
| 8   | AU    | 102    |    |
| 9   | AO    | 134    |    |
| 10  | AX    | 143    |    |
| 11  | AM    | 119    |    |
| 12  | AS    | 137    |    |
| 13  | Ad    | 52     |    |
| 14  | AN    | 150    |    |
| 15  | AL    | 155    |    |
| 16  | AR    | 120    |  |
| 17  | AP    | 124    |  |
| 18  | AV    | 82     |  |
| 19  | AY    | 126    |  |
| 20  | AZ    | 74     |  |
| 21  | Aa    | 107    |  |
| 22  | Ab    | 84     |  |
| 23  | AD    | 227    |  |
| 24  | Ae    | 58     |  |
| 25  | Af    | 80     |  |
| 26  | AJ    | 181    |  |
| 27  | Ca    | 149    |  |
| 28  | CN    | 203    |  |

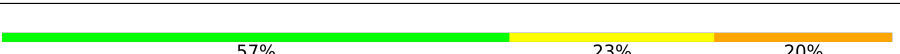
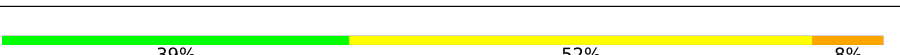
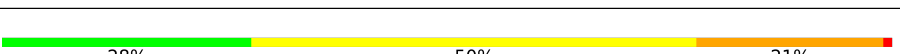
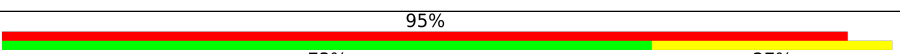
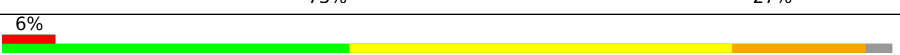
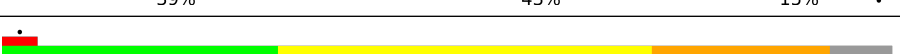
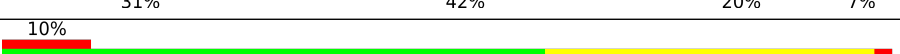
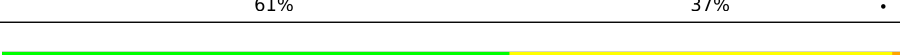
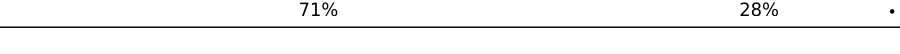
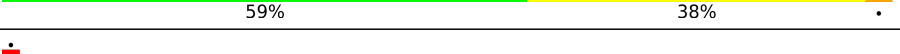
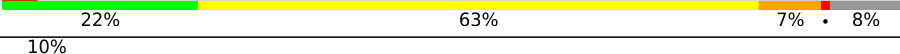
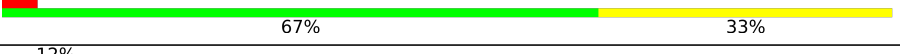
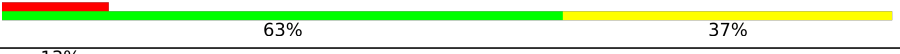
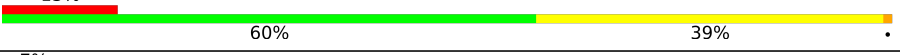
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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 29  | CI    | 217    |    |
| 30  | CD    | 290    |    |
| 31  | CQ    | 187    |    |
| 32  | CR    | 203    |    |
| 33  | CS    | 173    |    |
| 34  | CT    | 158    |    |
| 35  | CP    | 185    |    |
| 36  | CX    | 120    |    |
| 37  | CY    | 131    |    |
| 38  | CZ    | 134    |    |
| 39  | Cr    | 134    |    |
| 40  | Ch    | 123    |  |
| 41  | Cb    | 75     |  |
| 42  | Cc    | 100    |  |
| 43  | Cd    | 111    |  |
| 44  | Ce    | 132    |  |
| 45  | Cf    | 157    |  |
| 46  | Ci    | 113    |  |
| 47  | Ck    | 70     |  |
| 48  | Cl    | 50     |  |
| 49  | Cm    | 52     |  |
| 50  | Cn    | 25     |  |
| 51  | Cp    | 91     |  |
| 52  | Co    | 104    |  |
| 53  | CJ    | 182    |  |

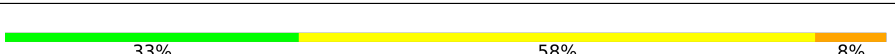
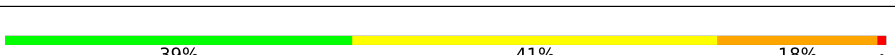
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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 54  | CH    | 190    |    |
| 55  | CE    | 228    |    |
| 56  | CG    | 241    |    |
| 57  | A9    | 30     |    |
| 58  | A7    | 120    |    |
| 59  | A8    | 123    |    |
| 60  | Cz    | 217    |    |
| 61  | B2    | 1995   |    |
| 62  | A5    | 3974   |    |
| 63  | Ac    | 62     |    |
| 64  | AW    | 129    |    |
| 65  | CW    | 58     |    |
| 66  | Cg    | 104    |   |
| 67  | CU    | 96     |  |
| 68  | AK    | 90     |  |
| 69  | AT    | 143    |  |
| 70  | AF    | 189    |  |
| 71  | CF    | 226    |  |
| 72  | AE    | 261    |  |
| 73  | AG    | 231    |  |
| 74  | AH    | 194    |  |
| 75  | AI    | 207    |  |
| 76  | AQ    | 148    |  |
| 77  | CO    | 205    |  |
| 78  | CL    | 210    |  |

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| Mol | Chain | Length | Quality of chain                                                                   |
|-----|-------|--------|------------------------------------------------------------------------------------|
| 79  | CV    | 134    |  |
| 80  | CM    | 159    |  |
| 81  | B     | 75     |  |
| 82  | v     | 12     |  |
| 83  | Cj    | 87     |  |

## 2 Entry composition

There are 83 unique types of molecules in this entry. The entry contains 219005 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 40S ribosomal protein SA.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 1   | AA    | 218      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1737  | 1113 | 298 | 321 | 5 |         |       |

- Molecule 2 is a protein called 60S ribosomal protein L8.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 2   | CA    | 253      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1935  | 1206 | 395 | 326 | 8 |         |       |

- Molecule 3 is a protein called 40S ribosomal protein S3a.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 3   | AB    | 220      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1798  | 1138 | 328 | 324 | 8 |         |       |

- Molecule 4 is a protein called 60S ribosomal protein L3.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 4   | CB    | 414      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3287  | 2083 | 621 | 565 | 18 |         |       |

- Molecule 5 is a protein called 40S ribosomal protein S2.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 5   | AC    | 227      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1746  | 1126 | 302 | 311 | 7 |         |       |

- Molecule 6 is a protein called 60S ribosomal protein L4.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 6   | CC    | 392      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 3109  | 1959 | 622 | 522 | 6 |         |       |

- Molecule 7 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 7   | Ag    | 318      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2511  | 1577 | 444 | 480 | 10 |         |       |

- Molecule 8 is a protein called 40S ribosomal protein S20.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 8   | AU    | 102      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 815   | 505 | 161 | 145 | 4 |         |       |

- Molecule 9 is a protein called 40S ribosomal protein S14a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 9   | AO    | 134      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1003  | 616 | 196 | 187 | 4 |         |       |

- Molecule 10 is a protein called 40S ribosomal protein S23.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 10  | AX    | 143      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1131  | 712 | 226 | 191 | 2 |         |       |

- Molecule 11 is a protein called 40S ribosomal protein S12.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 11  | AM    | 119      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 924   | 582 | 165 | 171 | 6 |         |       |

- Molecule 12 is a protein called 40S ribosomal protein S18.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 12  | AS    | 137      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1128  | 707 | 220 | 198 | 3 |         |       |

- Molecule 13 is a protein called 40S ribosomal protein S29.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 13  | Ad    | 52       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 433   | 269 | 87 | 72 | 5 |         |       |

- Molecule 14 is a protein called 40S ribosomal protein S13.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 14  | AN    | 150      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1202  | 767 | 229 | 203 | 3 |         |       |

- Molecule 15 is a protein called 40S ribosomal protein S11.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 15  | AL    | 155      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1274  | 803 | 254 | 211 | 6 |         |       |

- Molecule 16 is a protein called 40S ribosomal protein S17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 16  | AR    | 120      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 981   | 618 | 183 | 176 | 4 |         |       |

- Molecule 17 is a protein called GEO07301p1.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 17  | AP    | 124      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1016  | 652 | 189 | 169 | 6 |         |       |

- Molecule 18 is a protein called 40S ribosomal protein S21.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 18  | AV    | 82       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 617   | 373 | 114 | 125 | 5 |         |       |

There are 13 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| AV    | 2       | GLN      | GLU    | conflict | UNP O76927 |
| AV    | 8       | PHE      | ASN    | conflict | UNP O76927 |
| AV    | 25      | GLY      | HIS    | conflict | UNP O76927 |
| AV    | 32      | ILE      | VAL    | conflict | UNP O76927 |
| AV    | 34      | MET      | LEU    | conflict | UNP O76927 |
| AV    | 35      | ASN      | SER    | conflict | UNP O76927 |
| AV    | 36      | VAL      | ILE    | conflict | UNP O76927 |
| AV    | 58      | ALA      | GLU    | conflict | UNP O76927 |
| AV    | 68      | SER      | CYS    | conflict | UNP O76927 |
| AV    | 70      | LEU      | VAL    | conflict | UNP O76927 |
| AV    | 75      | ALA      | LYS    | conflict | UNP O76927 |
| AV    | 79      | VAL      | ILE    | conflict | UNP O76927 |

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| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| AV    | 80      | SER      | THR    | conflict | UNP O76927 |

- Molecule 19 is a protein called 40S ribosomal protein S24.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 19  | AY    | 126      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1016  | 644 | 196 | 171 | 5 |         |       |

- Molecule 20 is a protein called 40S ribosomal protein S25.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 20  | AZ    | 74       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 608   | 390 | 112 | 106 |   |         |       |

- Molecule 21 is a protein called 40S ribosomal protein S26.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 21  | Aa    | 107      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 867   | 539 | 182 | 140 | 6 |         |       |

- Molecule 22 is a protein called 40S ribosomal protein S27.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 22  | Ab    | 84       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 653   | 412 | 123 | 110 | 8 |         |       |

- Molecule 23 is a protein called 40S ribosomal protein S3.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 23  | AD    | 227      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1782  | 1127 | 319 | 326 | 10 |         |       |

- Molecule 24 is a protein called 40S ribosomal protein S30.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 24  | Ae    | 58       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 469   | 289 | 105 | 75 |   |         |       |

- Molecule 25 is a protein called Ubiquitin-40S ribosomal protein S27a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 25  | Af    | 80       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 659   | 417 | 128 | 109 | 5 |         |       |

- Molecule 26 is a protein called 40S ribosomal protein S9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 26  | AJ    | 181      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1503  | 957 | 298 | 247 | 1 |         |       |

- Molecule 27 is a protein called 60S ribosomal protein L27a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 27  | Ca    | 149      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1204  | 769 | 242 | 189 | 4 |         |       |

- Molecule 28 is a protein called 60S ribosomal protein L15.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 28  | CN    | 203      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1710  | 1072 | 362 | 271 | 5 |         |       |

- Molecule 29 is a protein called 60S ribosomal protein L10.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 29  | CI    | 217      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1785  | 1125 | 343 | 304 | 13 |         |       |

- Molecule 30 is a protein called 60S ribosomal protein L5.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 30  | CD    | 290      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2334  | 1471 | 434 | 423 | 6 |         |       |

- Molecule 31 is a protein called 60S ribosomal protein L18.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 31  | CQ    | 187      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1518  | 957 | 306 | 251 | 4 |         |       |

- Molecule 32 is a protein called 60S ribosomal protein L19.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 32  | CR    | 203      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1683  | 1047 | 350 | 277 | 9 |         |       |

- Molecule 33 is a protein called 60S ribosomal protein L18a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 33  | CS    | 173      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1454  | 935 | 275 | 240 | 4 |         |       |

- Molecule 34 is a protein called RE62581p.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 34  | CT    | 158      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1297  | 829 | 253 | 212 | 3 |         |       |

- Molecule 35 is a protein called 60S ribosomal protein L17.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 35  | CP    | 185      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1505  | 928 | 305 | 263 | 9 |         |       |

- Molecule 36 is a protein called IP17216p.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 36  | CX    | 120      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 984   | 625 | 192 | 165 | 2 |         |       |

- Molecule 37 is a protein called GEO07453p1.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 37  | CY    | 131      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1078  | 676 | 224 | 176 | 2 |         |       |

- Molecule 38 is a protein called 60S ribosomal protein L27.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 38  | CZ    | 134      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1115  | 723 | 209 | 180 | 3 |         |       |

- Molecule 39 is a protein called 60S ribosomal protein L28.

| Mol | Chain | Residues | Atoms |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 39  | Cr    | 134      | Total | C   | N   | O   | 0       | 0     |
|     |       |          | 1051  | 670 | 205 | 176 |         |       |

- Molecule 40 is a protein called FI02809p.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 40  | Ch    | 123      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1015  | 646 | 202 | 164 | 3 |         |       |

- Molecule 41 is a protein called 60S ribosomal protein L29.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 41  | Cb    | 75       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 619   | 378 | 133 | 107 | 1 |         |       |

- Molecule 42 is a protein called RE25263p.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 42  | Cc    | 100      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 770   | 486 | 132 | 147 | 5 |         |       |

- Molecule 43 is a protein called 60S ribosomal protein L31.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 43  | Cd    | 111      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 924   | 573 | 180 | 169 | 2 |         |       |

- Molecule 44 is a protein called 60S ribosomal protein L32.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 44  | Ce    | 132      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1110  | 698 | 230 | 177 | 5 |         |       |

- Molecule 45 is a protein called GEO07455p1.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 45  | Cf    | 157      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1244  | 781 | 255 | 203 | 5 |         |       |

- Molecule 46 is a protein called 60S ribosomal protein L36.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 46  | Ci    | 113      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 934   | 585 | 193 | 153 | 3 |         |       |

- Molecule 47 is a protein called 60S ribosomal protein L38.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 47  | Ck    | 70       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 576   | 366 | 108 | 100 | 2 |         |       |

- Molecule 48 is a protein called 60S ribosomal protein L39.

| Mol | Chain | Residues | Atoms |     |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|-------|
| 48  | Cl    | 50       | Total | C   | N  | O  | 0       | 0     |
|     |       |          | 437   | 276 | 98 | 63 |         |       |

- Molecule 49 is a protein called Ubiquitin-60S ribosomal protein L40.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 49  | Cm    | 52       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 429   | 267 | 89 | 67 | 6 |         |       |

- Molecule 50 is a protein called 60S ribosomal protein L41.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 50  | Cn    | 25       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 236   | 143 | 63 | 27 | 3 |         |       |

- Molecule 51 is a protein called 60S ribosomal protein L37a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 51  | Cp    | 91       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 710   | 441 | 140 | 122 | 7 |         |       |

- Molecule 52 is a protein called TA01007p.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 52  | Co    | 104      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 874   | 548 | 180 | 138 | 8 |         |       |

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

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 53  | CJ    | 182      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1468  | 926 | 278 | 258 | 6 |         |       |

- Molecule 54 is a protein called 60S ribosomal protein L9.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 54  | CH    | 190      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1499  | 947 | 265 | 278 | 9 |         |       |

- Molecule 55 is a protein called Ribosomal protein L6, isoform A.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 55  | CE    | 228      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1845  | 1185 | 351 | 305 | 4 |         |       |

- Molecule 56 is a protein called 60S ribosomal protein L7a.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 56  | CG    | 241      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1936  | 1237 | 368 | 327 | 4 |         |       |

- Molecule 57 is a RNA chain called 2S ribosomal RNA.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 57  | A9    | 30       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 639   | 286 | 111 | 213 | 29 |         |       |

- Molecule 58 is a RNA chain called 5S ribosomal RNA.

| Mol | Chain | Residues | Atoms |      |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
| 58  | A7    | 120      | Total | C    | N   | O   | P   | 0       | 0     |
|     |       |          | 2554  | 1141 | 456 | 838 | 119 |         |       |

- Molecule 59 is a RNA chain called 5.8S ribosomal RNA.

| Mol | Chain | Residues | Atoms |      |     |     |     | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|-------|
| 59  | A8    | 123      | Total | C    | N   | O   | P   | 0       | 0     |
|     |       |          | 2621  | 1173 | 474 | 852 | 122 |         |       |

- Molecule 60 is a protein called 60S ribosomal protein L10a-2.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 60  | Cz    | 217      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1702  | 1084 | 303 | 305 | 10 |         |       |

- Molecule 61 is a RNA chain called 18S ribosomal RNA.

| Mol | Chain | Residues | Atoms |       |      |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|-------|
| 61  | B2    | 1936     | Total | C     | N    | O     | P    | 0       | 0     |
|     |       |          | 39355 | 17526 | 6780 | 13114 | 1935 |         |       |

- Molecule 62 is a RNA chain called 28S ribosomal RNA.

| Mol | Chain | Residues | Atoms |       |       |       |      | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|-------|
| 62  | A5    | 3707     | Total | C     | N     | O     | P    | 0       | 0     |
|     |       |          | 77175 | 34473 | 13566 | 25431 | 3705 |         |       |

There are 10 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment   | Reference      |
|-------|---------|----------|--------|-----------|----------------|
| A5    | 1301    | A        | U      | conflict  | GB NR_133562.1 |
| A5    | 1319    | A        | U      | conflict  | GB NR_133562.1 |
| A5    | 1320    | U        | G      | conflict  | GB NR_133562.1 |
| A5    | 1321    | G        | U      | conflict  | GB NR_133562.1 |
| A5    | 1322    | U        | G      | conflict  | GB NR_133562.1 |
| A5    | 1686    | A        | -      | insertion | GB NR_133562.1 |
| A5    | 1710    | G        | -      | insertion | GB NR_133562.1 |
| A5    | 2158A   | C        | -      | insertion | GB NR_133562.1 |
| A5    | 2279    | C        | G      | conflict  | GB NR_133562.1 |
| A5    | 3569    | C        | -      | insertion | GB NR_133562.1 |

- Molecule 63 is a protein called 40S ribosomal protein S28.

| Mol | Chain | Residues | Atoms |     |     |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|-------|
| 63  | Ac    | 62       | Total | C   | N   | O  | S | 0       | 0     |
|     |       |          | 498   | 307 | 100 | 89 | 2 |         |       |

- Molecule 64 is a protein called 40S ribosomal protein S15Aa.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 64  | AW    | 129      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1028  | 656 | 189 | 176 | 7 |         |       |

- Molecule 65 is a protein called 60S ribosomal protein L24.

| Mol | Chain | Residues | Atoms |     |    |    |   | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 65  | CW    | 58       | Total | C   | N  | O  | S | 0       | 0     |
|     |       |          | 483   | 314 | 89 | 76 | 4 |         |       |

- Molecule 66 is a protein called RH48056p.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 66  | Cg    | 104      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 852   | 530 | 177 | 139 | 6 |         |       |

- Molecule 67 is a protein called Ribosomal protein L22-like protein.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 67  | CU    | 96       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 811   | 531 | 137 | 139 | 4 |         |       |

- Molecule 68 is a protein called 40S ribosomal protein S10b.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 68  | AK    | 90       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 760   | 500 | 130 | 127 | 3 |         |       |

- Molecule 69 is a protein called 40S ribosomal protein S19a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 69  | AT    | 132      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1041  | 659 | 200 | 179 | 3 |         |       |

- Molecule 70 is a protein called 40S ribosomal protein S5a.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 70  | AF    | 189      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1490  | 929 | 284 | 268 | 9 |         |       |

- Molecule 71 is a protein called 60S ribosomal protein L7.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 71  | CF    | 226      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1895  | 1216 | 368 | 308 | 3 |         |       |

- Molecule 72 is a protein called 40S ribosomal protein S4.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 72  | AE    | 261      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 2054  | 1314 | 380 | 353 | 7 |         |       |

- Molecule 73 is a protein called 40S ribosomal protein S6.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 73  | AG    | 231      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1866  | 1172 | 372 | 315 | 7 |         |       |

- Molecule 74 is a protein called 40S ribosomal protein S7.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 74  | AH    | 194      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1566  | 1006 | 278 | 281 | 1 |         |       |

- Molecule 75 is a protein called 40S ribosomal protein S8.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 75  | AI    | 207      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1665  | 1037 | 329 | 296 | 3 |         |       |

- Molecule 76 is a protein called 40S ribosomal protein S16.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 76  | AQ    | 148      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1183  | 753 | 223 | 204 | 3 |         |       |

- Molecule 77 is a protein called 60S ribosomal protein L13a.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 77  | CO    | 205      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1668  | 1063 | 331 | 268 | 6 |         |       |

- Molecule 78 is a protein called 60S ribosomal protein L13.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 78  | CL    | 210      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1695  | 1066 | 342 | 284 | 3 |         |       |

- Molecule 79 is a protein called 60S ribosomal protein L23.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 79  | CV    | 134      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 998   | 629 | 190 | 173 | 6 |         |       |

- Molecule 80 is a protein called 60S ribosomal protein L14.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 80  | CM    | 159      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1302  | 826 | 256 | 218 | 2 |         |       |

- Molecule 81 is a RNA chain called P-tRNA.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 81  | B     | 75       | Total | C   | N   | O   | P  | 0       | 0     |
|     |       |          | 1605  | 717 | 296 | 518 | 74 |         |       |

- Molecule 82 is a RNA chain called mRNA.

| Mol | Chain | Residues | Atoms |     |    |    |    | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|----|---------|-------|
| 82  | v     | 12       | Total | C   | N  | O  | P  | 0       | 0     |
|     |       |          | 255   | 113 | 43 | 87 | 12 |         |       |

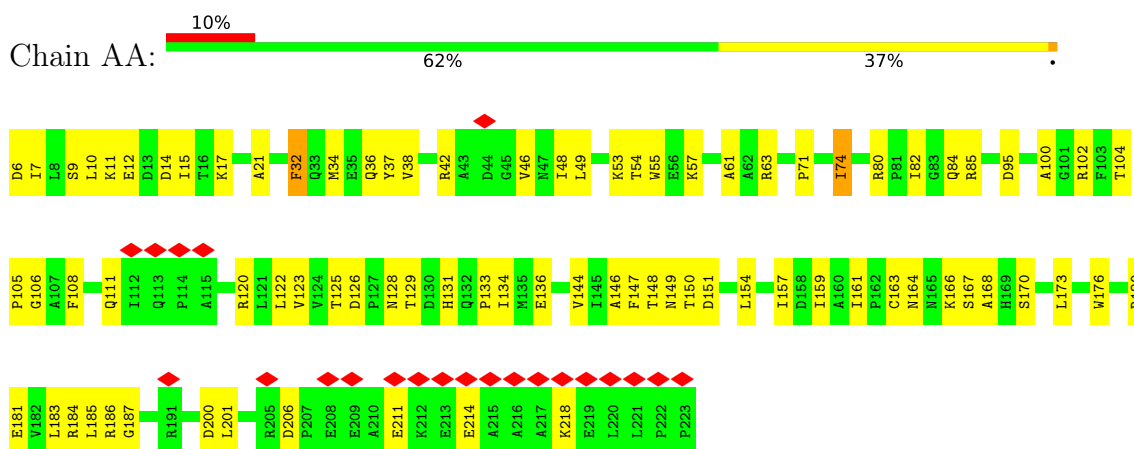
- Molecule 83 is a protein called Probable 60S ribosomal protein L37-B.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 83  | Cj    | 87       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 696   | 422 | 154 | 115 | 5 |         |       |

### 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.

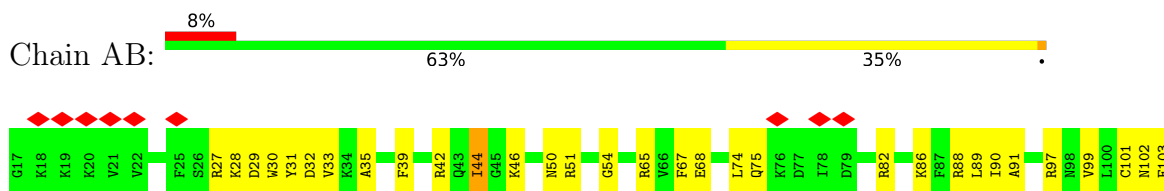
- Molecule 1: 40S ribosomal protein SA

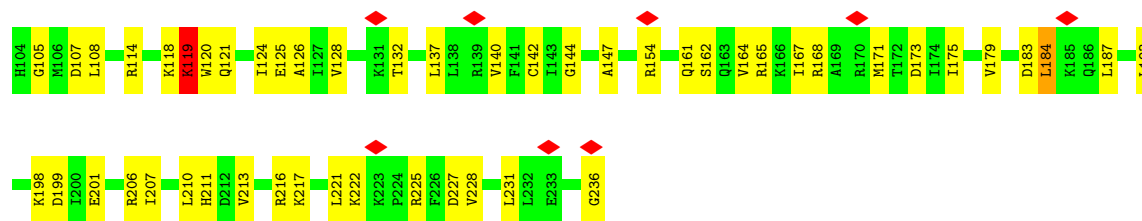


- Molecule 2: 60S ribosomal protein L8



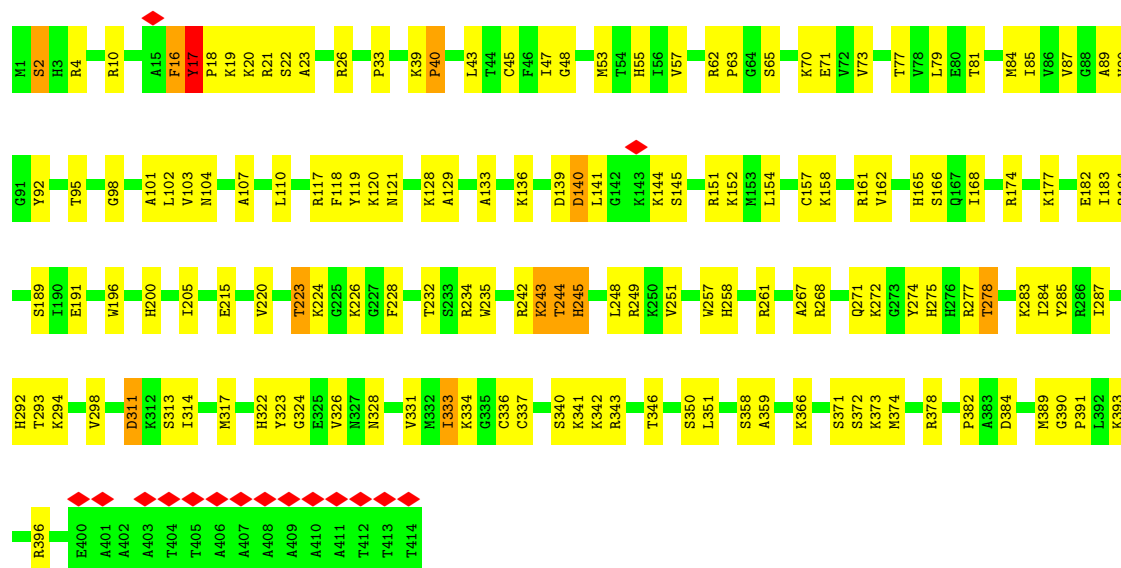
- Molecule 3: 40S ribosomal protein S3a





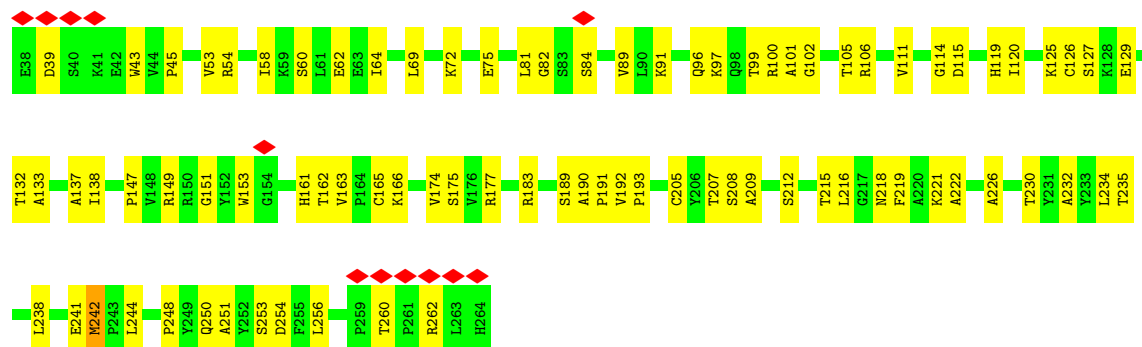
• Molecule 4: 60S ribosomal protein L3

Chain CB: 64% 33%



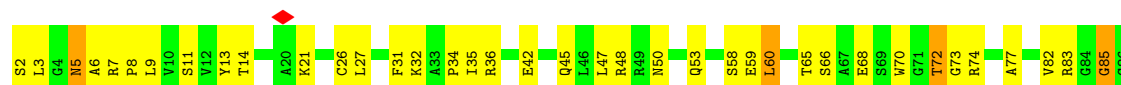
• Molecule 5: 40S ribosomal protein S2

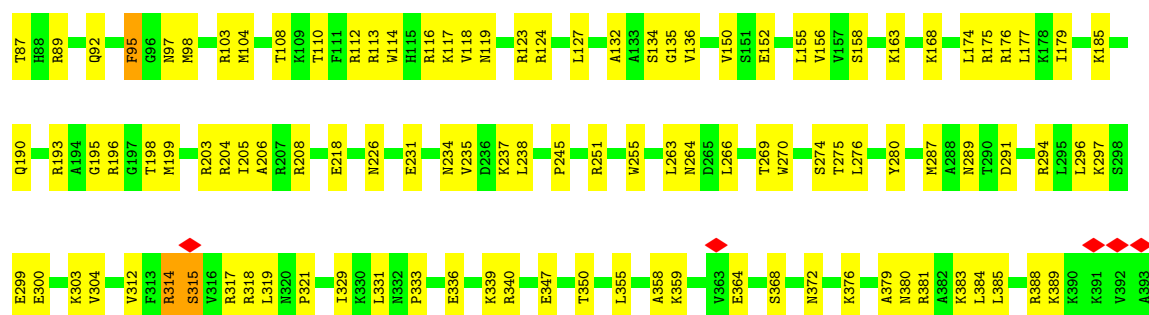
Chain AC: 5% 63% 37%



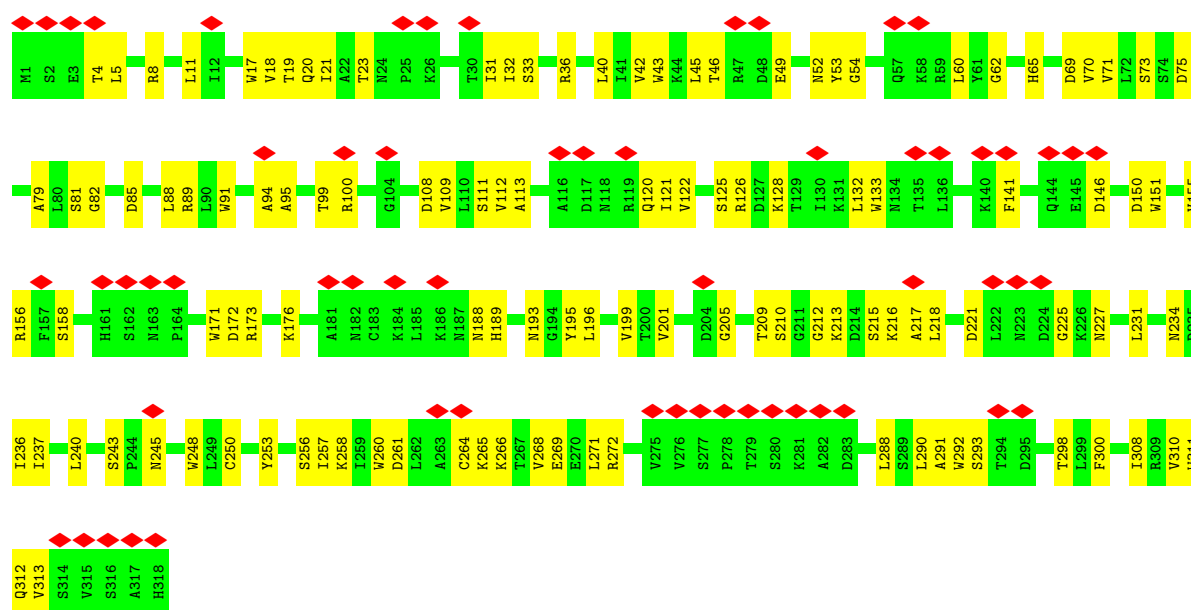
• Molecule 6: 60S ribosomal protein L4

Chain CC: 63% 35%

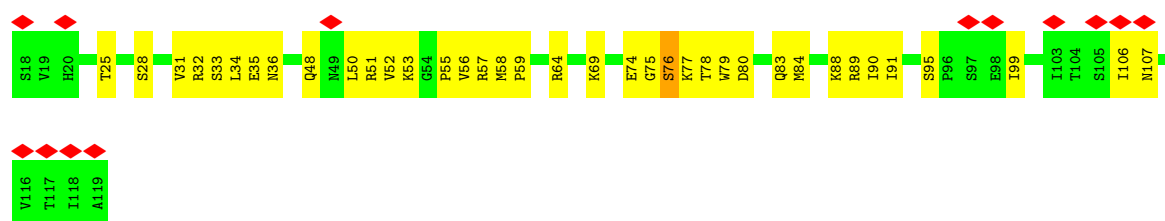




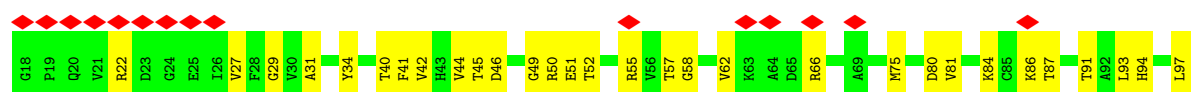
• Molecule 7: Guanine nucleotide-binding protein subunit beta-like protein

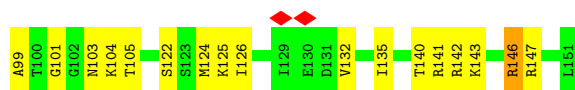


• Molecule 8: 40S ribosomal protein S20



• Molecule 9: 40S ribosomal protein S14a





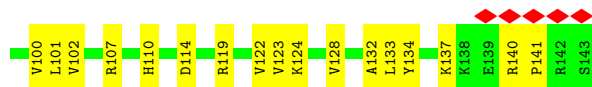
- Molecule 10: 40S ribosomal protein S23

Chain AX: 62% 38%



- Molecule 11: 40S ribosomal protein S12

Chain AM: 61% 38%



- Molecule 12: 40S ribosomal protein S18

Chain AS: 58% 42%



- Molecule 13: 40S ribosomal protein S29

Chain Ad: 58% 38%

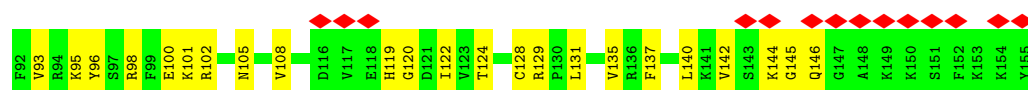
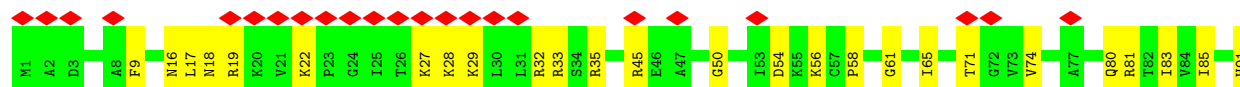


- Molecule 14: 40S ribosomal protein S13

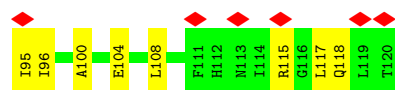
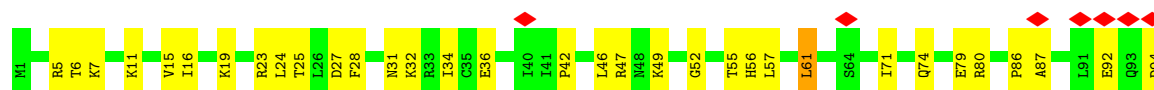
Chain AN: 66% 34%



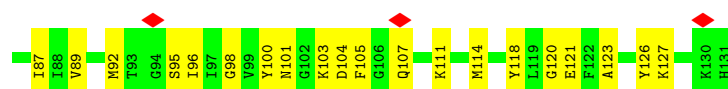
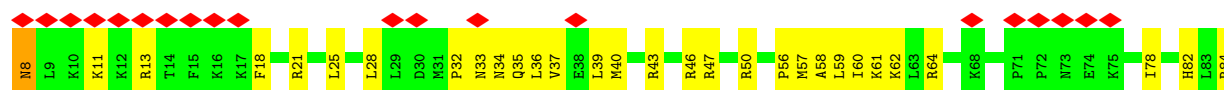
• Molecule 15: 40S ribosomal protein S11



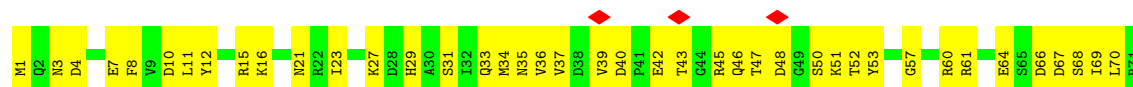
• Molecule 16: 40S ribosomal protein S17

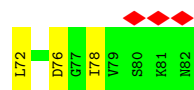


• Molecule 17: GEO07301p1



• Molecule 18: 40S ribosomal protein S21





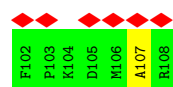
- Molecule 19: 40S ribosomal protein S24



- Molecule 20: 40S ribosomal protein S25



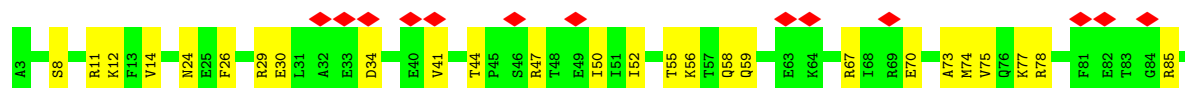
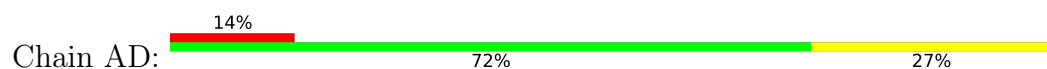
- Molecule 21: 40S ribosomal protein S26

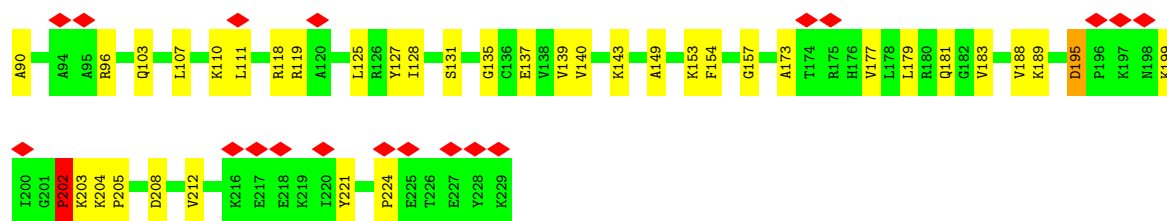


- Molecule 22: 40S ribosomal protein S27

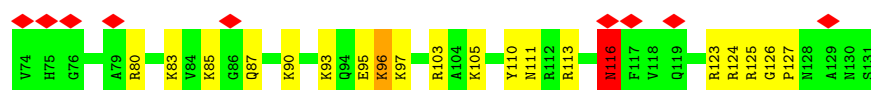


- Molecule 23: 40S ribosomal protein S3

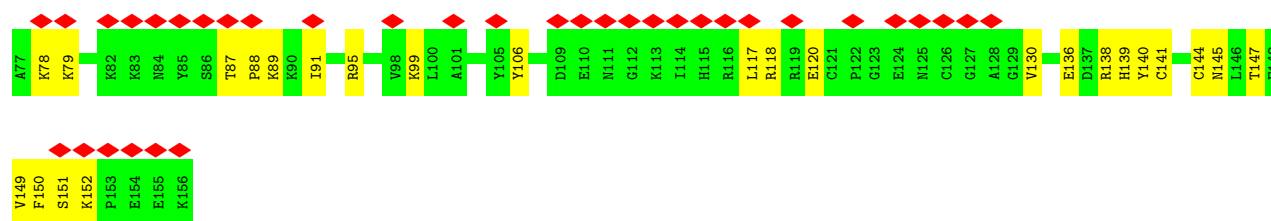




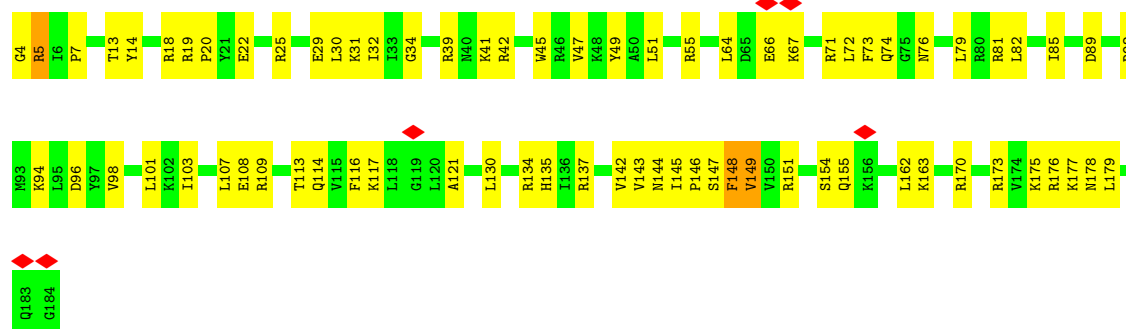
- Molecule 24: 40S ribosomal protein S30



- Molecule 25: Ubiquitin-40S ribosomal protein S27a

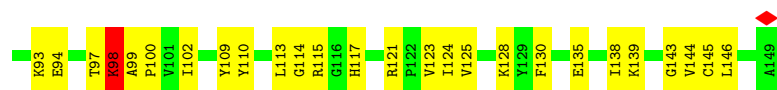


- Molecule 26: 40S ribosomal protein S9

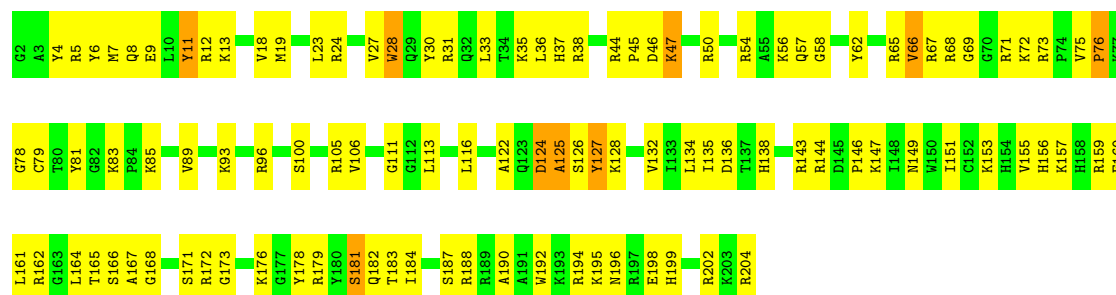


- Molecule 27: 60S ribosomal protein L27a

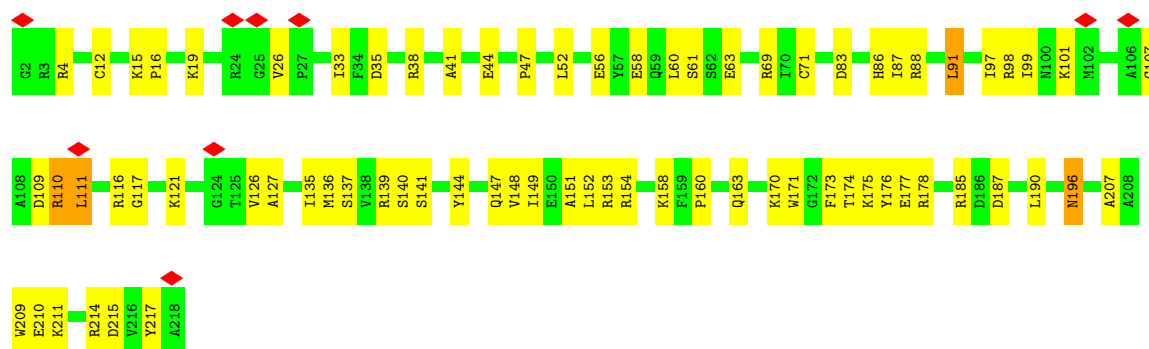




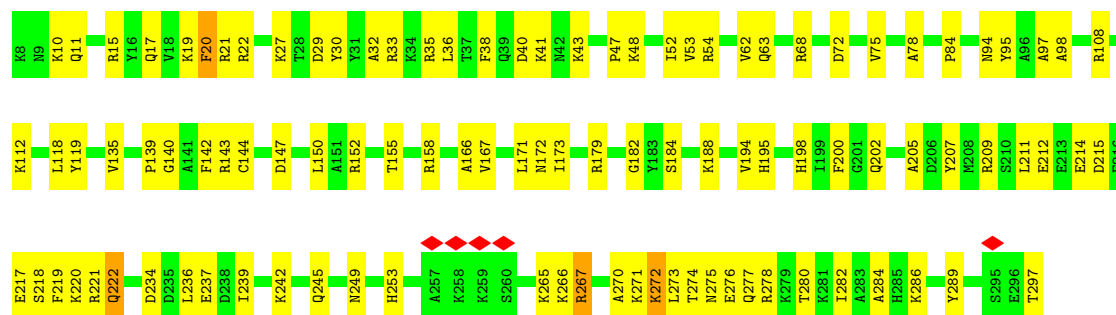
• Molecule 28: 60S ribosomal protein L15



• Molecule 29: 60S ribosomal protein L10

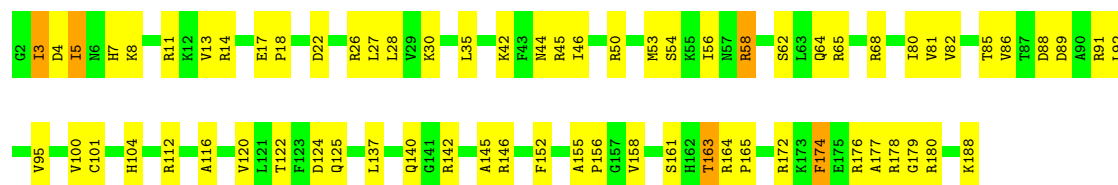


• Molecule 30: 60S ribosomal protein L5

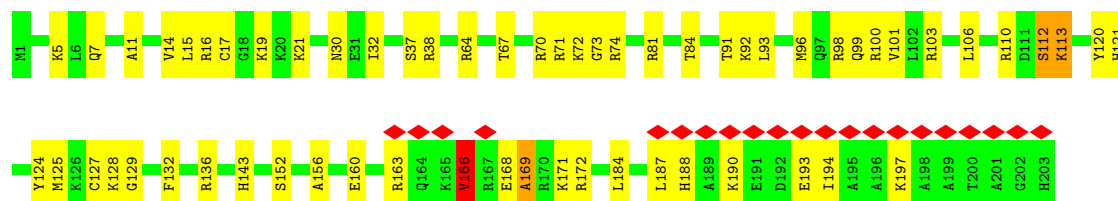
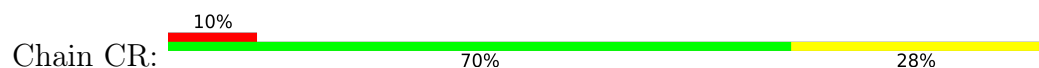


• Molecule 31: 60S ribosomal protein L18

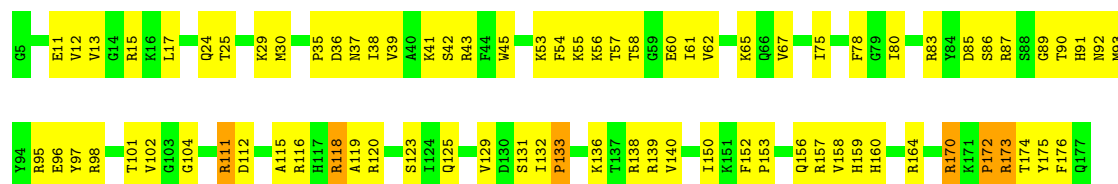




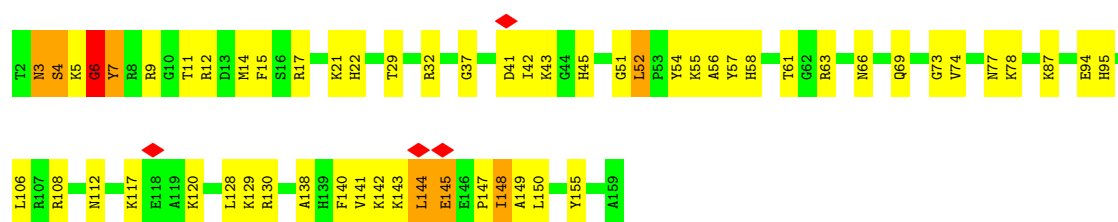
• Molecule 32: 60S ribosomal protein L19



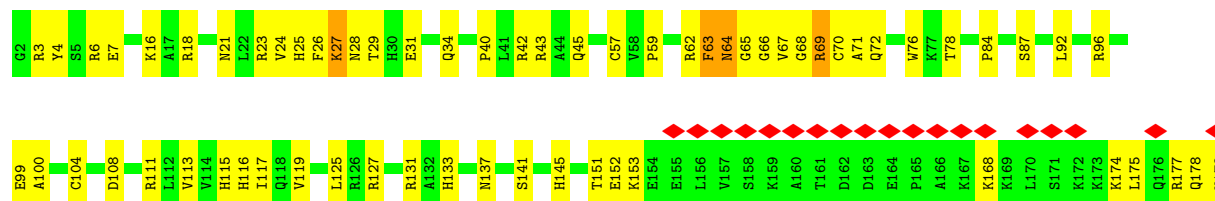
• Molecule 33: 60S ribosomal protein L18a

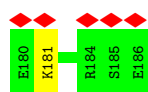


• Molecule 34: RE62581p



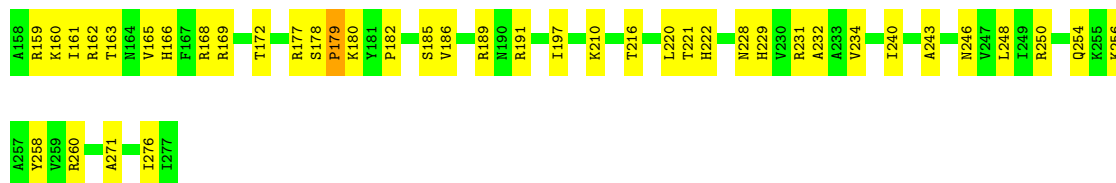
• Molecule 35: 60S ribosomal protein L17





• Molecule 36: IP17216p

Chain CX: 66% 33%



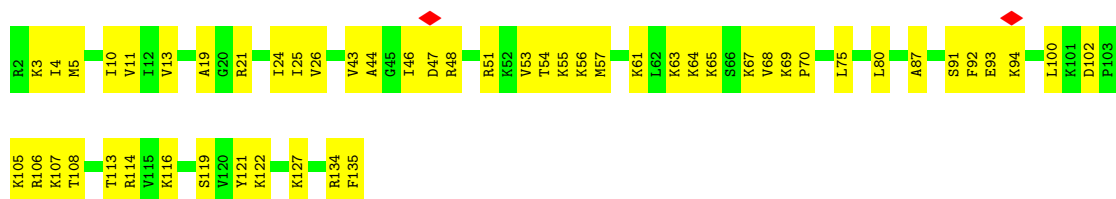
• Molecule 37: GEO07453p1

Chain CY: 69% 31%



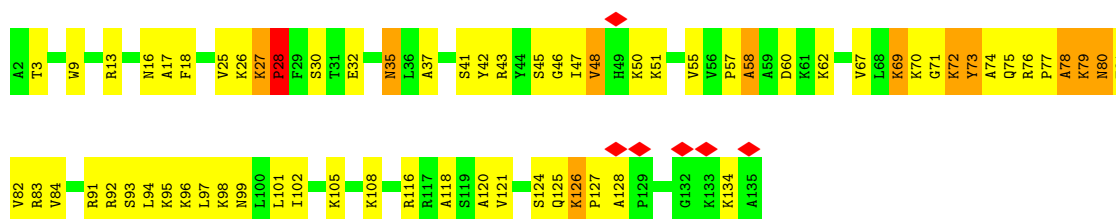
• Molecule 38: 60S ribosomal protein L27

Chain CZ: 60% 40%



• Molecule 39: 60S ribosomal protein L28

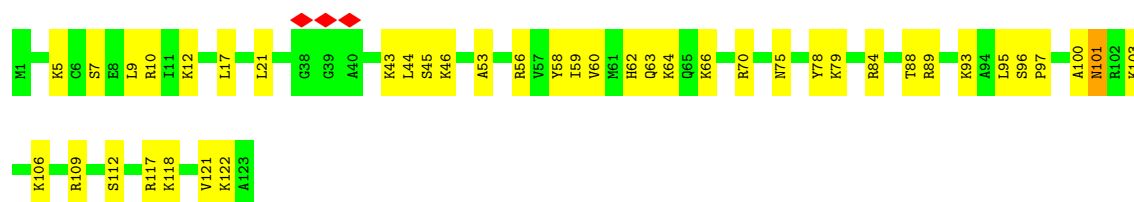
Chain Cr: 49% 42% 8%



• Molecule 40: FI02809p

Chain Ch: 67% 33%





- Molecule 41: 60S ribosomal protein L29

Chain Cb: 71% 25% ..



- Molecule 42: RE25263p

Chain Cc: 69% 30% .



- Molecule 43: 60S ribosomal protein L31

Chain Cd: 68% 30% .



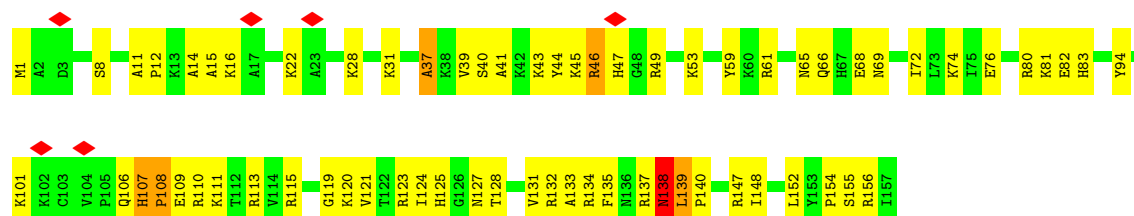
- Molecule 44: 60S ribosomal protein L32

Chain Ce: 66% 30% ..

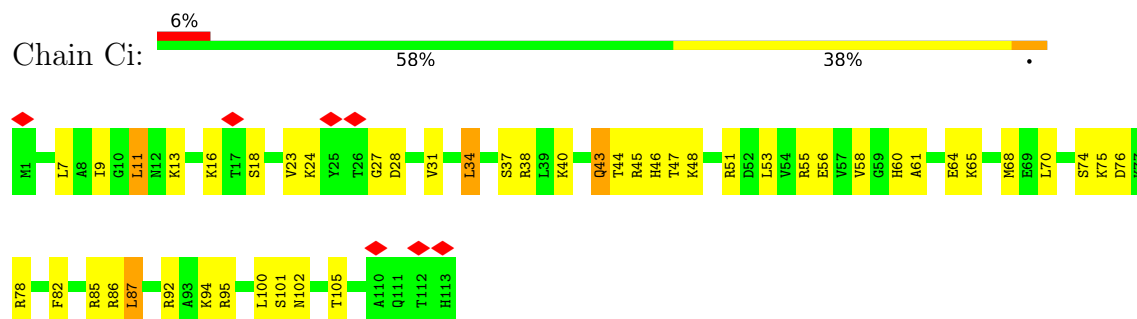


- Molecule 45: GEO07455p1

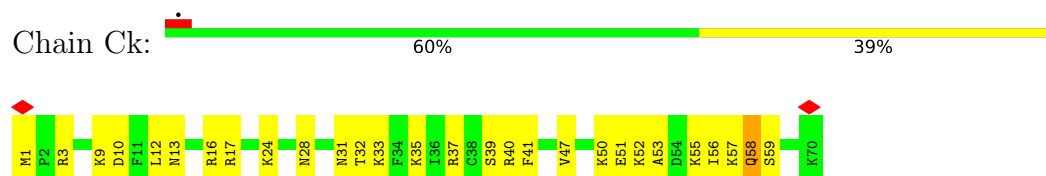
Chain Cf: 57% 39% ..



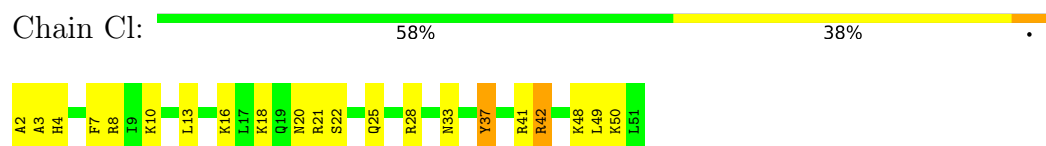
- Molecule 46: 60S ribosomal protein L36



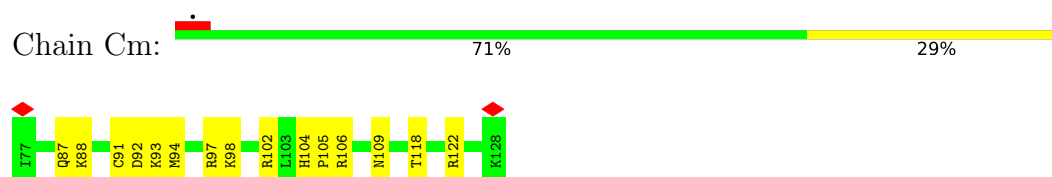
- Molecule 47: 60S ribosomal protein L38



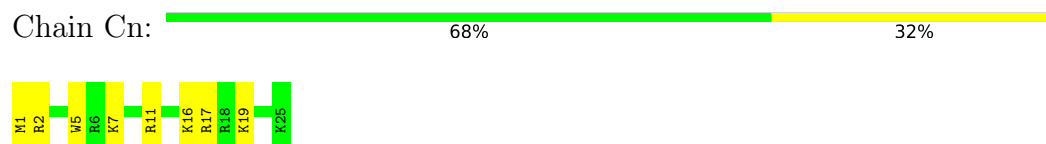
- Molecule 48: 60S ribosomal protein L39



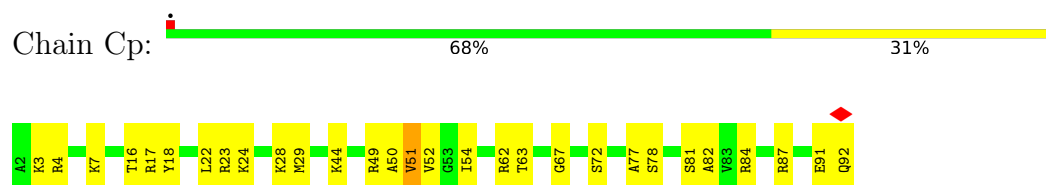
- Molecule 49: Ubiquitin-60S ribosomal protein L40



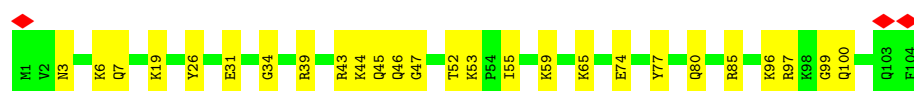
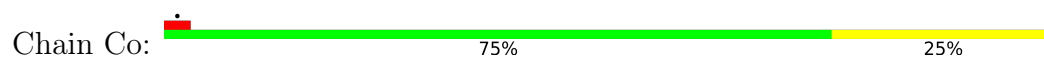
- Molecule 50: 60S ribosomal protein L41



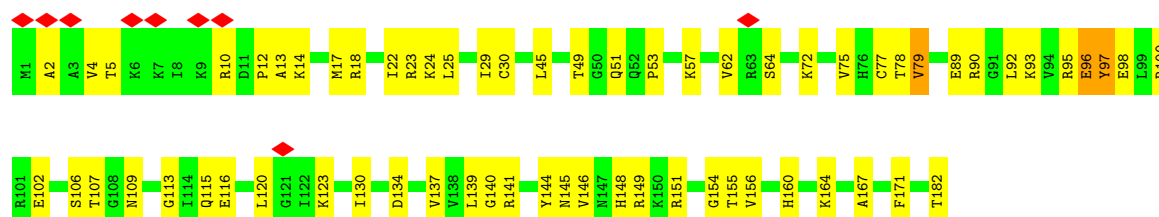
- Molecule 51: 60S ribosomal protein L37a



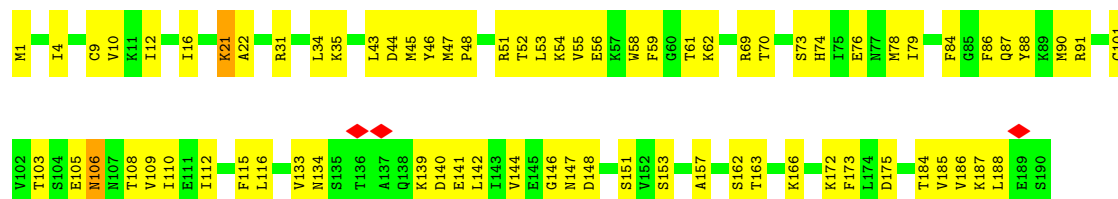
- Molecule 52: TA01007p



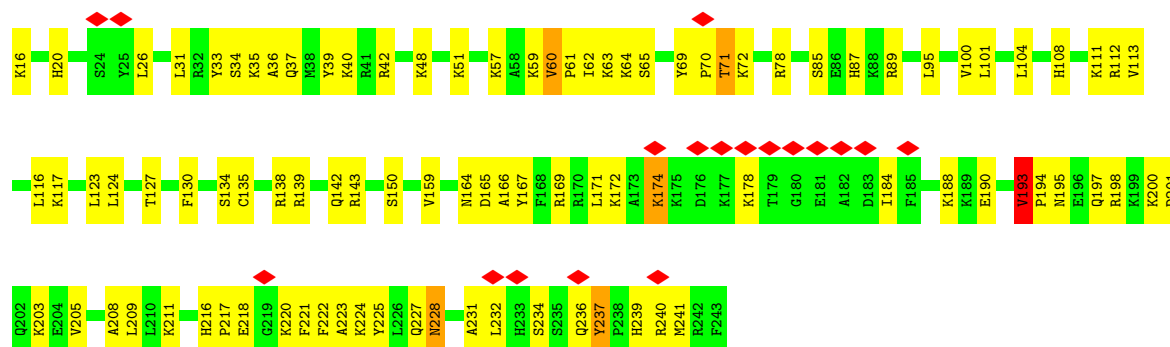
• Molecule 53: 60S ribosomal protein L11



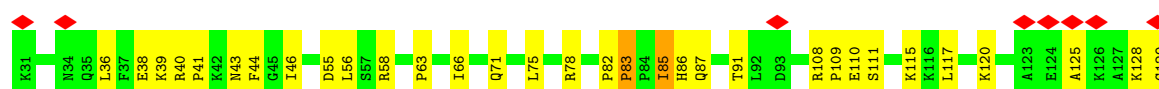
• Molecule 54: 60S ribosomal protein L9

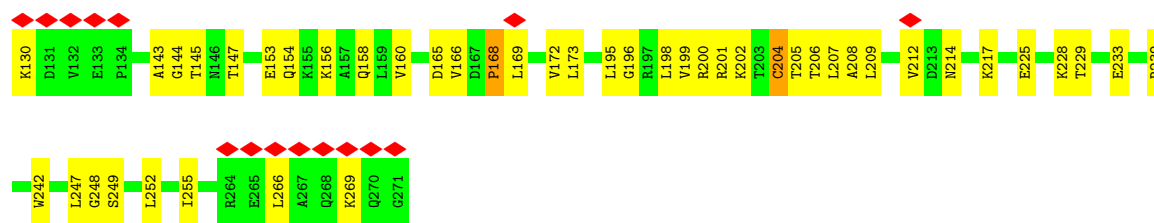


• Molecule 55: Ribosomal protein L6, isoform A

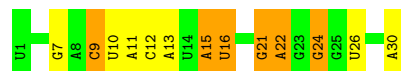


• Molecule 56: 60S ribosomal protein L7a

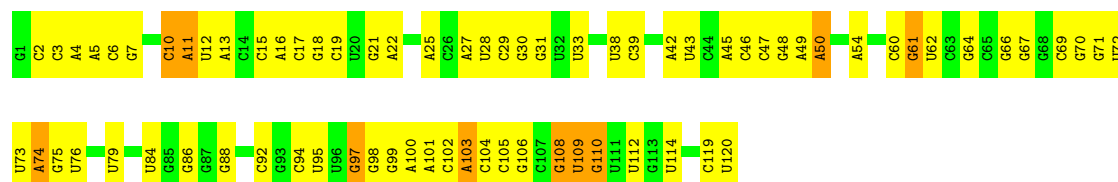




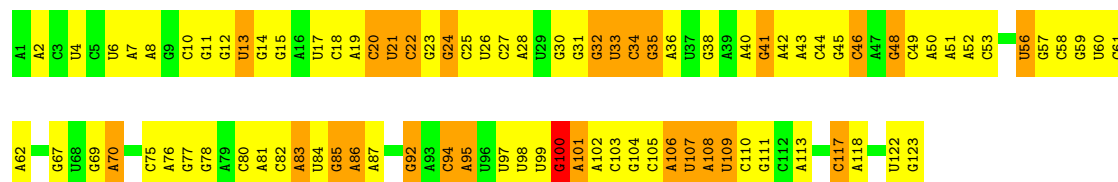
• Molecule 57: 2S ribosomal RNA



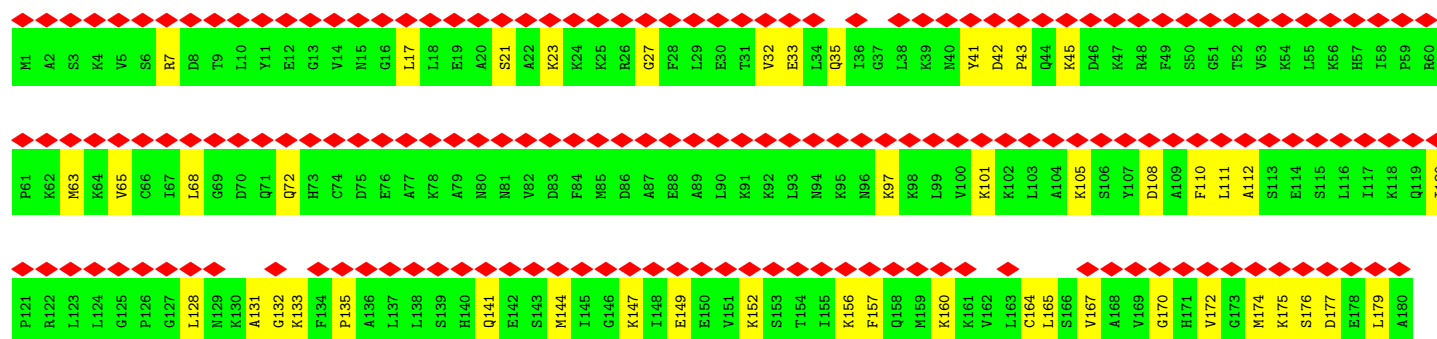
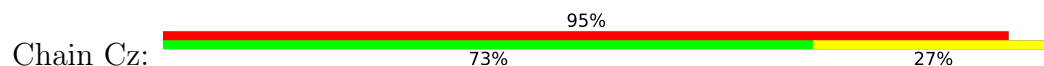
• Molecule 58: 5S ribosomal RNA



• Molecule 59: 5.8S ribosomal RNA

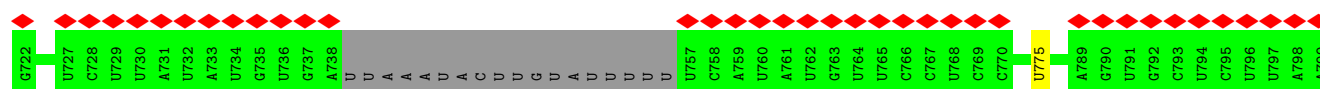
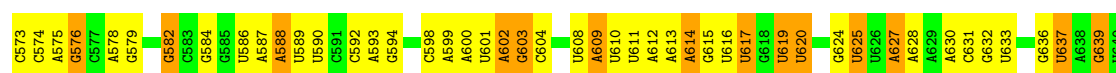
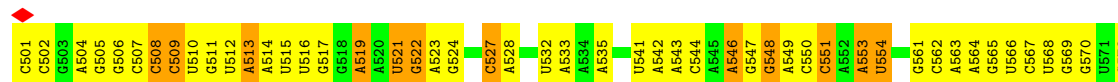
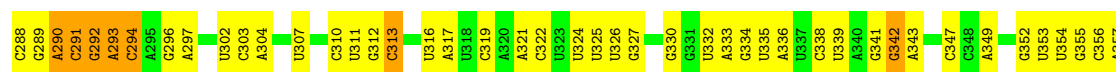
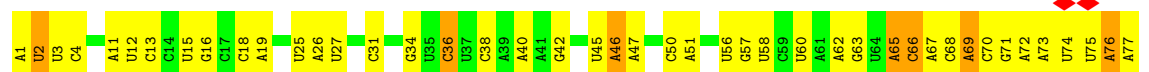


• Molecule 60: 60S ribosomal protein L10a-2

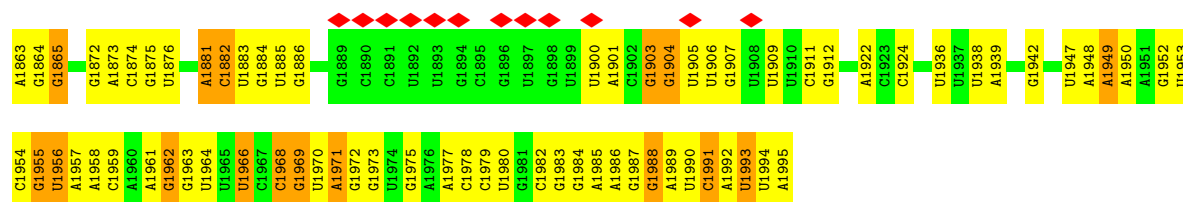




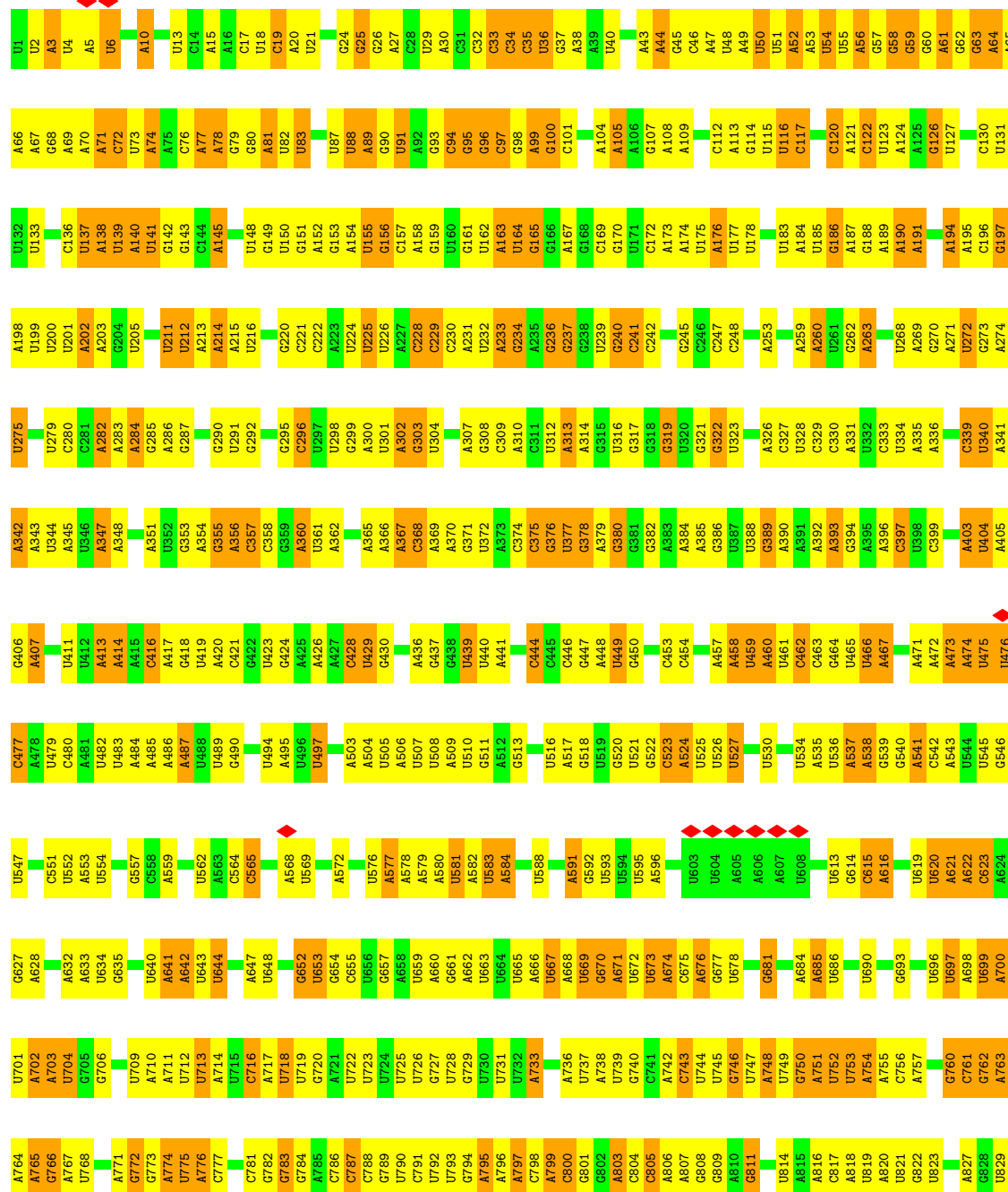
• Molecule 61: 18S ribosomal RNA



|       |       |       |       |       |       |       |       |       |       |       |      |      |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|------|
| U1783 | A1717 | C1582 | U1507 | U1434 | U1353 | A1290 | G1219 | G1151 | A1088 | A1017 | A935 | A872 |
| G1786 | C1718 | A1583 | U1508 | A1435 | G1354 | A1291 | A1220 | G1152 | G1089 | A1018 | G936 | A873 |
| U1787 | C1719 | A1584 | U1509 | G1436 | A1362 | A1292 | A1221 | C1157 | G1090 | U1019 | A937 | U874 |
| C1788 | U1654 | A1585 | U1510 | U1438 | U1363 | C1293 | C1222 | U1158 | U1091 | C1018 | G938 | A875 |
|       | U1722 | U1586 |       |       |       | U1294 | U1224 | C1159 | A1092 | U1020 | G939 | U876 |
|       | U1723 | U1587 |       |       |       | A1296 | U1225 | A1160 | A1022 | A1021 | U940 | U877 |
| A1793 | U1723 | G1588 | U1513 | C1441 | C1367 |       | A1226 | G1161 | G1093 | A1022 | A941 | C878 |
| C1794 | U1724 | C1589 | G1514 | U1442 | G1368 |       | A1227 | G1162 | C1094 | C1023 | A942 | U879 |
| U1795 | C1725 | G1590 |       | U1443 | U1371 |       | A1230 | G1164 | C1095 | C1024 | U943 | G880 |
| C1797 | A1661 | U1591 | A1520 | A1445 | U1372 |       |       | C1165 | C1096 | G1025 | A944 | U881 |
|       |       | C1592 |       | G1446 | A1374 |       |       | U1166 | C1097 | A1026 | A945 | G882 |
| A1798 | U1664 | U1592 | U1527 | G1447 | U1375 |       |       | U1167 | A1028 | A1027 | U946 | U885 |
| C1799 | A1594 | G1593 | G1528 | U1448 | G1376 |       |       | C1168 | G1029 | A1028 | A946 | G886 |
| U1800 | G1595 | U1594 | G1529 | A1449 |       |       |       | C1169 | C1030 | A1030 | A949 | G887 |
| U1801 | A1667 | A1596 | A1530 | U1450 |       |       |       | G1170 | A1031 | U1032 | U950 | G888 |
| G1802 | C1668 | A1597 | G1531 | A1451 | C1378 |       |       | G1171 | A106  | A1032 | A951 | A889 |
| A1803 | U1669 | A1598 | C1532 | U1452 | U1379 |       |       | C1172 | A107  | A1038 | G952 | U890 |
| U1804 | G1670 | A1599 | C1533 | G1453 | U1380 |       |       | A1173 | C1037 | A1038 | A953 | A891 |
| U1805 | A1671 | U1599 | G1534 |       | G1381 |       |       | A1174 | A1039 | A1039 | A954 | A892 |
|       | A1601 | U1535 | U1535 | C1457 | A1383 |       |       | A1175 | A1040 | A1040 | A957 |      |
| G1808 | U1673 | A1602 | U1536 | U1458 | G1384 |       |       | A1176 | A1041 | A1041 | A958 | A895 |
| U1809 | C1674 | G1603 | U1539 | A1459 | U1385 |       |       | A1177 | A1042 | A1042 | A959 | A896 |
| C1810 | A1675 | A1604 | G1540 | A1460 | G1386 |       |       | A1178 | A1043 | A1043 | U960 | A897 |
| C1811 |       | G1605 | U1541 |       | U1387 |       |       | A1179 |       |       | U961 | U898 |
| G1812 | U1678 | A1606 | U1542 | U1467 | U1388 |       |       | A1180 |       |       | U962 | A899 |
| U1813 | U1679 |       |       | G1468 |       |       |       |       |       |       | G962 | A900 |
| G1814 | G1680 |       | U1543 |       | U1392 |       |       |       |       |       | G963 | G901 |
| C1815 | U1681 |       | G1544 |       | C1393 |       |       |       |       |       | G964 | A902 |
| C1816 | A1682 |       | U1545 |       | U1394 |       |       |       |       |       |      | C903 |
| C1817 | U1683 |       | U1546 |       |       |       |       |       |       |       |      | C904 |
| U1818 | U1684 |       |       |       |       |       |       |       |       |       |      | U905 |
| U1819 | U1685 |       | U1547 | A1477 | U1398 |       |       |       |       |       |      | U906 |
| U1820 | C1686 |       | G1548 | U1478 | A1399 |       |       |       |       |       |      | U907 |
| G1821 | U1616 |       | U1549 | U1479 | A1400 |       |       |       |       |       |      | G908 |
| U1822 | A1617 |       | C1550 |       | U1401 |       |       |       |       |       |      | U909 |
| A1823 | C1618 |       | C1551 | C     |       |       |       |       |       |       |      | C911 |
| C1824 | U1619 |       | U1552 | A     | C1404 |       |       |       |       |       |      | U912 |
| A1825 | G1620 |       |       | U     | G1405 |       |       |       |       |       |      | G913 |
| C1826 | G1621 |       | U1557 | G     | A1406 |       |       |       |       |       |      | U914 |
| A1827 | U1622 |       | A1558 | U     | U1407 |       |       |       |       |       |      | U915 |
| C1828 | C1623 |       | A1559 | U     | A1408 |       |       |       |       |       |      | U916 |
| C1829 | U1624 |       | G1560 | C     | A1409 |       |       |       |       |       |      | U917 |
| G1830 | G1625 |       | G1561 | G     | C1410 |       |       |       |       |       |      | C918 |
| C1831 | U1626 |       | A1564 | C     | G1411 |       |       |       |       |       |      | A919 |
| C1832 | G1627 |       | C1565 | A     | A1412 |       |       |       |       |       |      | U920 |
| C1833 | A1628 |       | U1566 | U     |       |       |       |       |       |       |      | U921 |
| G1834 |       |       | A1567 | A     | G1415 |       |       |       |       |       |      | G922 |
|       |       |       | G1568 | A     | A1422 |       |       |       |       |       |      | G923 |
| U1839 | G1703 |       | C1569 | A     | A1423 |       |       |       |       |       |      | U926 |
|       | G1705 |       | U1570 | A     | A1424 |       |       |       |       |       |      | C928 |
| A1847 | U1706 |       | U1571 | U     | U1425 |       |       |       |       |       |      | U927 |
| U1848 | C1774 |       | C1572 | G     | A1426 |       |       |       |       |       |      | A929 |
| U1849 | A1708 |       | U1573 | U     | U1427 |       |       |       |       |       |      | G930 |
| G1850 | U1776 |       | U1574 | C     | A1428 |       |       |       |       |       |      | A931 |
| A1851 | A1709 |       | A1575 | U     | U1429 |       |       |       |       |       |      | U932 |
| C1852 |       |       | U1576 |       | U1430 |       |       |       |       |       |      | C933 |
| U1853 | G1712 |       | A1577 | A     | A1431 |       |       |       |       |       |      | A934 |
|       | C1713 |       | U1578 |       | U1432 |       |       |       |       |       |      |      |
|       | U1714 |       | G1579 |       | A1433 |       |       |       |       |       |      |      |
|       | G1715 |       | U1580 |       |       |       |       |       |       |       |      |      |
|       | A1716 |       | A1581 |       |       |       |       |       |       |       |      |      |



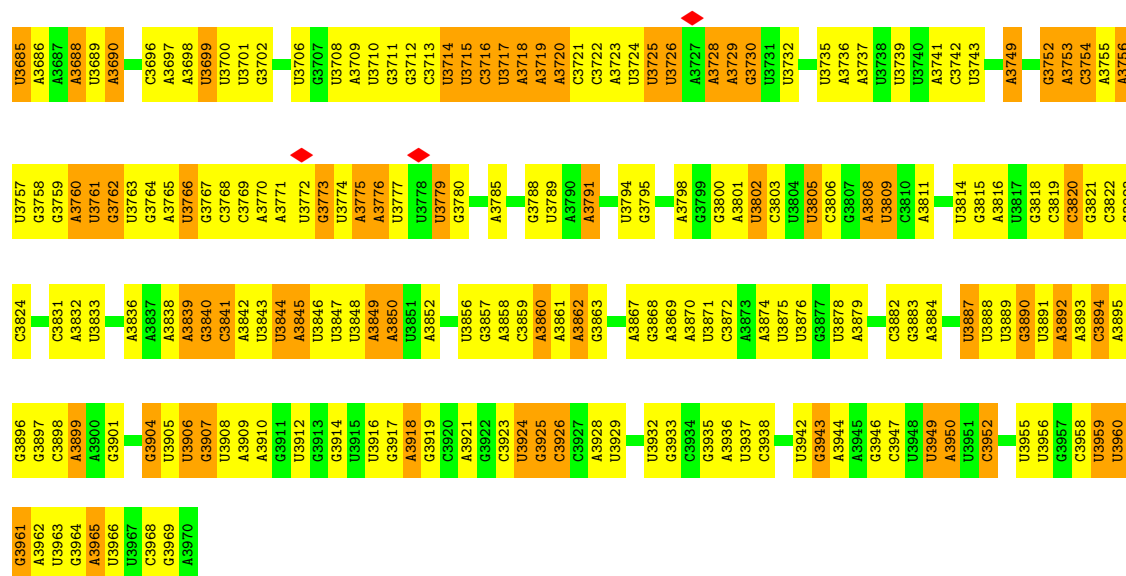
• Molecule 62: 28S ribosomal RNA



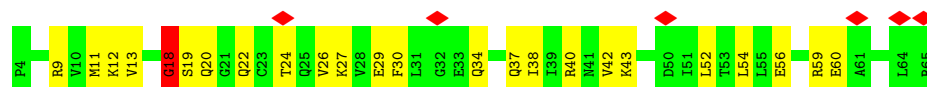
|      |      |      |       |       |       |       |       |       |       |       |       |       |       |      |      |      |       |       |       |       |       |       |       |       |       |       |      |      |      |       |       |       |       |       |       |       |       |       |       |       |      |      |      |       |       |       |       |       |       |       |       |       |       |       |      |      |      |       |       |       |       |       |       |       |       |       |       |       |      |      |      |       |       |       |       |       |       |       |       |       |       |      |      |      |       |       |       |       |       |       |       |       |       |       |       |      |      |      |       |       |       |       |       |       |       |       |       |       |       |      |      |      |       |       |       |       |       |       |       |       |       |       |       |      |      |      |       |      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|------|------|------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|------|------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|------|------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|------|------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|------|------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|------|------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|------|------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|------|------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|------|------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|------|------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|------|------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|------|------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|------|------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|------|------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|------|------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|------|------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|------|------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|------|------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|------|------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|------|------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|------|------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|------|------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|------|------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|------|------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|------|------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|------|------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|---|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| U830 | A802 | C981 | C1049 | A1113 | C1175 | A1253 | U1322 | U1387 | A1455 | G1522 | U1582 | C1651 | U1714 | U831 | U905 | U983 | C1050 | A1114 | U1176 | U1254 | U1323 | C1388 | U1456 | G1522 | U1582 | C1651 | U832 | U906 | U984 | C1051 | A1115 | U1177 | U1255 | U1324 | C1389 | U1457 | G1523 | U1583 | C1652 | U1715 | U833 | U907 | U985 | U1052 | A1116 | U1178 | U1256 | U1325 | C1390 | U1458 | G1524 | U1584 | C1653 | U1716 | U834 | U908 | U986 | U1053 | A1117 | U1179 | U1257 | U1326 | C1391 | U1459 | G1525 | U1585 | C1654 | U1717 | U835 | U909 | U987 | U1054 | A1118 | U1180 | U1258 | U1327 | C1392 | U1460 | U1586 | C1655 | U1718 | U836 | U910 | U988 | U1055 | C1119 | A1119 | U1181 | U1259 | U1328 | C1393 | U1461 | U1587 | C1656 | U1719 | U837 | U911 | U989 | U1056 | C1120 | A1121 | U1182 | U1260 | U1329 | C1394 | U1462 | U1588 | C1657 | U1720 | U838 | U912 | U990 | U1057 | C1121 | A1122 | U1183 | U1261 | U1330 | C1395 | U1463 | U1589 | C1658 | U1721 | U839 | U913 | U991 | U1058 | 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| U1263 | U1264 | U1265 | U1266 | U1267 | U1271 | U1272 | U1273 | U1274 | U1275 | U1276 | U1277 | U1278 | U1279 | U1280 | U1281 | U1282 | U1283 | U1284 | U1285 | U1286 | U1287 | U1288 | U1291 | U1292 | U1293 | U1294 | U1295 | U1296 | U1297 | U1298 | U1299 | U1300 | U1301 | U1305 | U1306 | U1307 | U1308 | U1309 | U1310 | U1311 | U1312 | U1313 | U1314 | U1315 | U1316 | U1317 | U1320 | U1321 | U1326 | U1327 | U1328 | U1329 | U1330 | U1331 | U1332 | U1333 | U1334 | U1339 | U1340 | U1341 | U1342 | U1343 | U1344 | U1345 | U1346 | U1347 | U1348 | U1349 | U1350 | U1351 | U1352 | U1353 | U1357 | U1358 | U1359 | U1360 | U1361 | U1362 | U1363 | U1364 | U1365 | U1366 | U1367 | U1368 | U1369 | U1372 | U1373 | U1374 | U1375 | U1376 | U1377 | U1378 | U1379 | U1380 | U1381 | U1382 | U1383 | U1384 | G | U1385 | U1386 | U1387 | U1388 | U1389 | U1390 | U1391 | U1392 | U1393 | U1394 | U1395 | U1396 | U1397 | U1398 | U1399 | U1400 | U1401 | U1402 | U1403 | U1404 | U1405 | U1406 | U1407 | U1408 | U1411 | U1412 | U1413 | U1414 | U1418 | U1421 | U1422 | U1423 | U1424 | U1425 | U1426 | U1427 | U1428 | U1429 | U1430 | U1431 | U1432 | U1435 | U1436 | U1437 | U1438 | U1442 | U1443 | U1446 | U1447 | U1448 | U1449 | U1450 | U1451 | U1452 | U1453 | U1454 | U1455 | U1456 | U1457 | U1458 | U1459 | U1460 | U1461 | U1462 | U1463 | U1464 | U1465 | U1466 | U1467 | U1468 | U1469 | U1470 | U1471 | U1472 | U1473 | U1474 | U1475 | U1476 | U1477 | U1478 | U1479 | U1480 | U1481 | U1483 | U1484 | U1485 | U1486 | U1487 | U1488 | U1489 | U1490 | U1491 | U1492 | U1493 | U1494 | U1499 | U1500 | U1501 | U1502 | U1503 | U1504 | U1505 | U1506 | U1507 | U1510 | U1511 | U1512 | U1513 | U1514 | U1515 | U1516 | U1517 | U1518 | U1519 | U1520 | U1521 | U1522 | U1523 | U1524 | U1525 | U1526 | U1527 | U1528 | U1529 | U1530 | U1531 | U1532 | U1533 | U1534 | U1535 | U1536 | U1537 | U1538 | U1539 | U1540 | U1541 | U1542 | U1543 | U1544 | U1545 | U1546 | U1547 | U1548 | U1549 | U1550 | U1551 | U1552 | U1553 | U1554 | U1555 | U1556 | U1557 | U1558 | U1559 | U1560 | U1561 | U1562 | U1563 | U1564 | U1565 | U1566 | U1567 | U1568 | U1569 | U1570 | U1571 | U1572 | U1573 | U1574 | U1575 | U1576 | U1577 | U1578 | U1579 | U1580 | U1581 | U1582 | U1583 | U1584 | U1585 | U1586 | U1587 | U1588 | U1589 | U1590 | U1591 | U1592 | U1593 | U1594 | U1595 | U1596 | U1597 | U1598 | U1599 | U1600 | U1601 | U1602 | U1603 | U1604 | U1605 | U1606 | U1607 | U1608 | U1609 | U1610 | U1611 | U1612 | U1613 | U1614 | U1615 | U1616 | U1617 | U1618 | U1619 | U1620 | U1621 | U1622 | U1623 | U1624 | U1627 | U1628 | U1629 | U1630 | U1631 | U1632 | U1633 | U1634 | U1635 | U1636 | U1640 | U1641 | U1642 | U1643 | U1644 | U1645 | U1646 | U1647 | U1650 | U1651 | U1652 | U1653 | U1654 | U1655 | U1656 | U1657 | U1658 | U1659 | U1660 | U1661 | U1662 | U1663 | U1664 | U1665 | U1666 | U1667 | U1668 | U1669 | U1670 | U1671 | U1672 | U1673 | U1674 | U1675 | U1676 | U1677 | U1678 | U1679 | U1680 | U1681 | U1682 | U1683 | U1684 | U1685 | U1686 | U1687 | U1688 | U1689 | U1690 | U1691 | U1692 | U1693 | U1694 | U1695 | U1696 | U1697 | U1698 | U1701 | U1702 | U1703 | U1704 | U1705 | U1706 | U1707 | U1708 | U1711 | U1712 | U1713 | U1714 | U1715 | U1716 | U1717 | U1718 | U1719 | U1720 | U1721 | U1722 | U1723 | U1724 | U1725 | U1726 | U1727 | U1731 | U1732 | U1733 | U1734 | U1735 | U1736 | U1737 | U1738 | U1739 | U1740 | U1741 | U1742 | U1743 | U1744 | U1745 | U1746 | U1747 | U1748 | U1749 | U1750 | U1751 | U1752 | U1753 | U1754 | U1755 | U1756 | U1757 | U1758 | U1759 | U1760 | U1761 | U1762 | U1763 | U1764 | U1765 | U1766 | U1767 | U1768 | U1769 | U1770 | U1771 | U1772 | U1773 | U1774 | U1775 | U1776 | U1777 | U1778 |
|------|------|------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|------|------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|------|------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|------|------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|------|------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|------|------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|------|------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|------|------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|------|------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|------|------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|------|------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|------|------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|------|------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|------|------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|------|------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|------|------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|------|------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|------|------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|------|------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|------|------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|------|------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|------|------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|------|------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|------|------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|------|------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|------|------|------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|---|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|







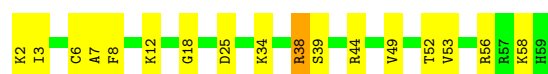
• Molecule 63: 40S ribosomal protein S28



• Molecule 64: 40S ribosomal protein S15Aa

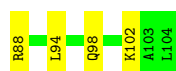


• Molecule 65: 60S ribosomal protein L24

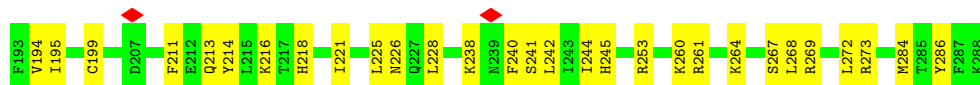


• Molecule 66: RH48056p

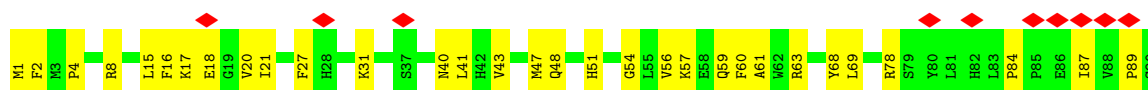




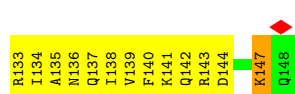
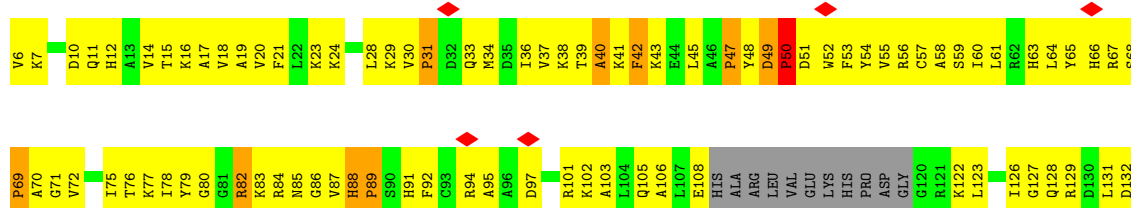
- Molecule 67: Ribosomal protein L22-like protein



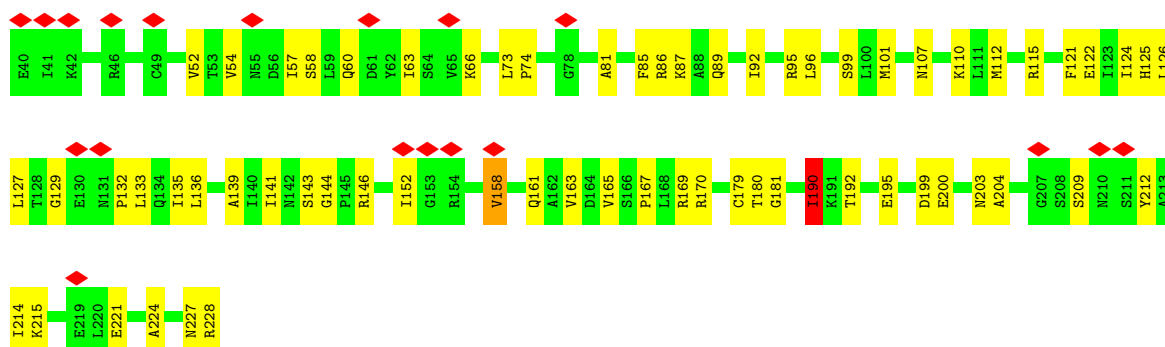
- Molecule 68: 40S ribosomal protein S10b



- Molecule 69: 40S ribosomal protein S19a

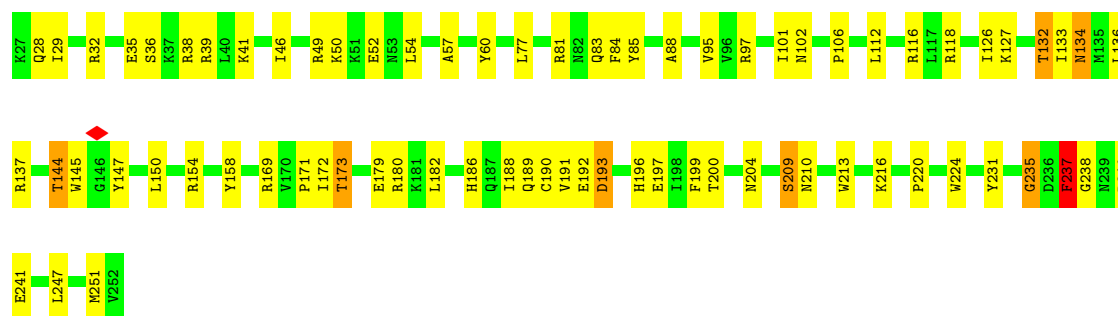


- Molecule 70: 40S ribosomal protein S5a



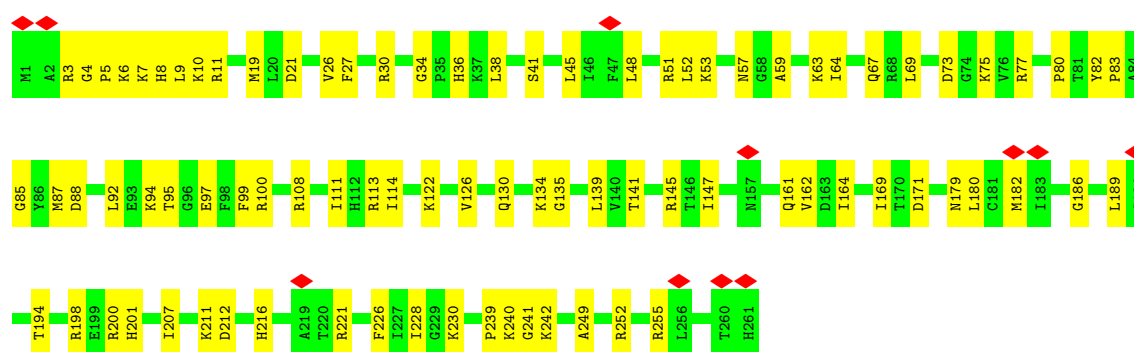
- Molecule 71: 60S ribosomal protein L7

Chain CF:  67% 30% .



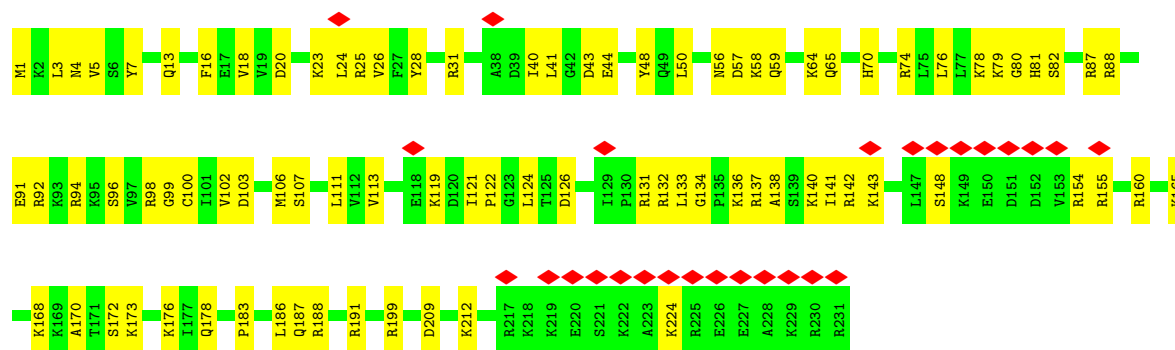
• Molecule 72: 40S ribosomal protein S4

Chain AE:  67% 33% .



• Molecule 73: 40S ribosomal protein S6

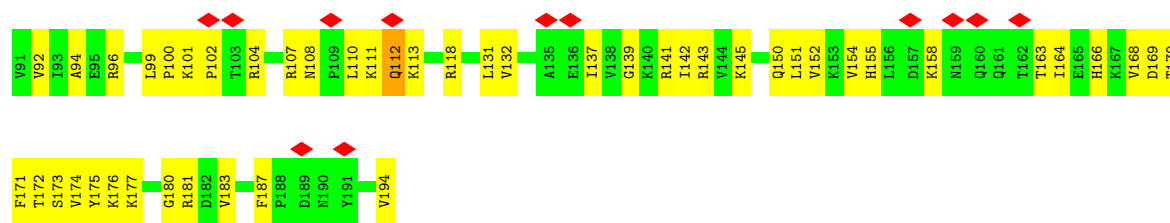
Chain AG:  12% 63% 37% .



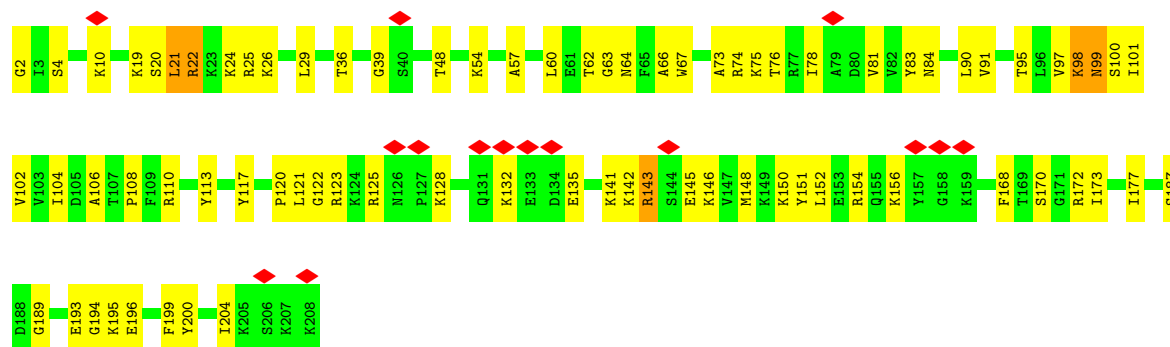
• Molecule 74: 40S ribosomal protein S7

Chain AH:  13% 60% 39% .

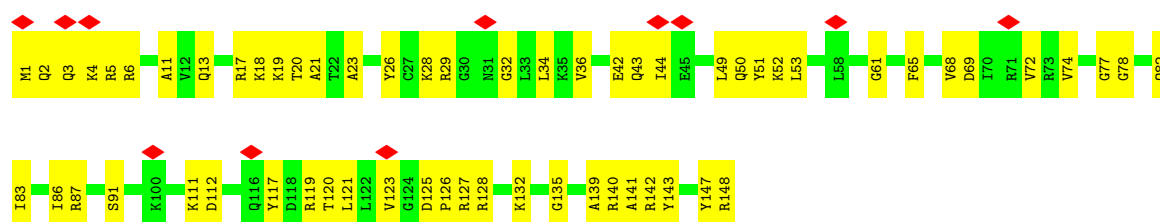




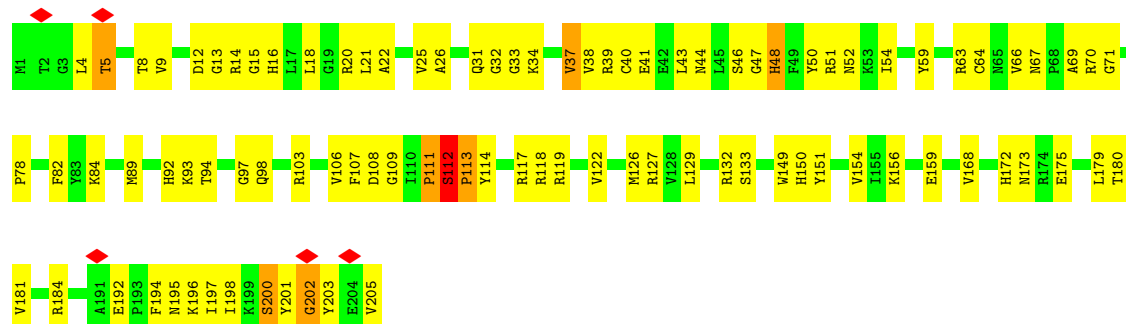
- Molecule 75: 40S ribosomal protein S8



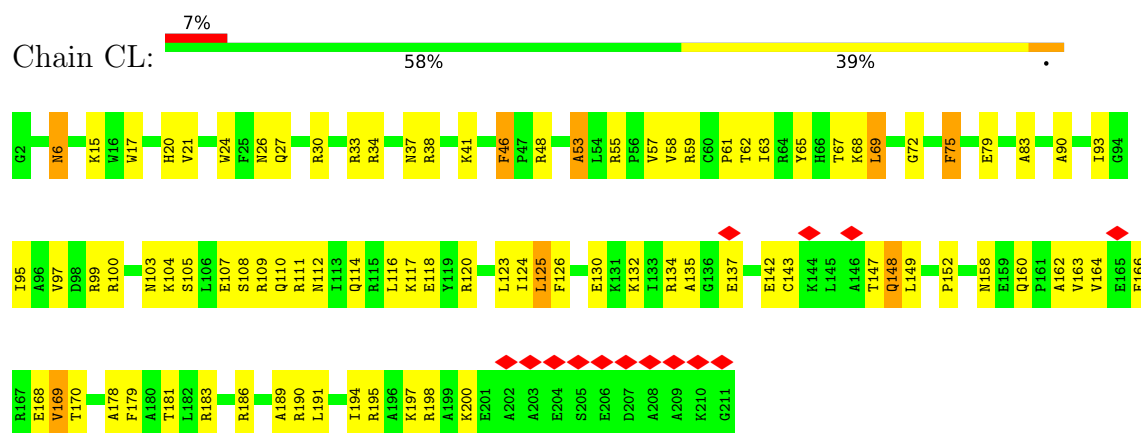
- Molecule 76: 40S ribosomal protein S16



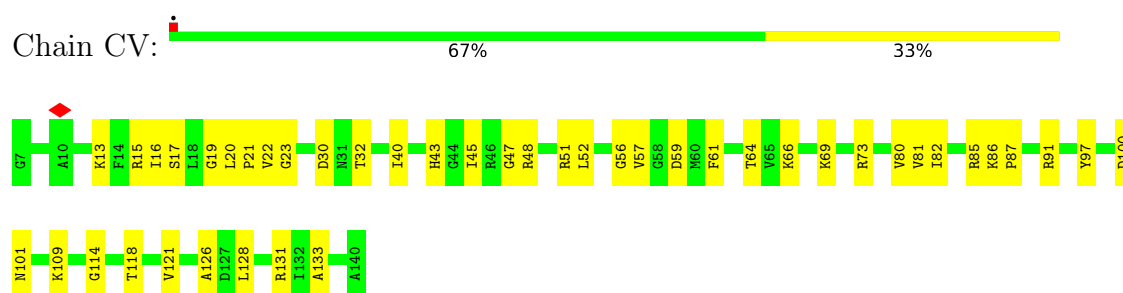
- Molecule 77: 60S ribosomal protein L13a



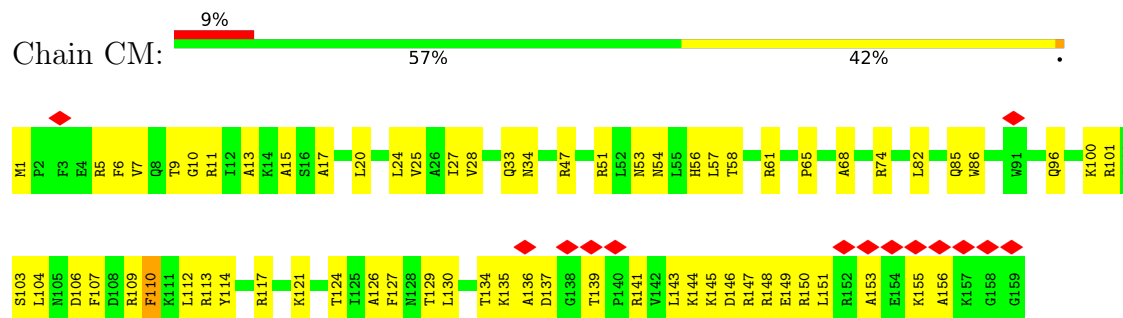
- Molecule 78: 60S ribosomal protein L13



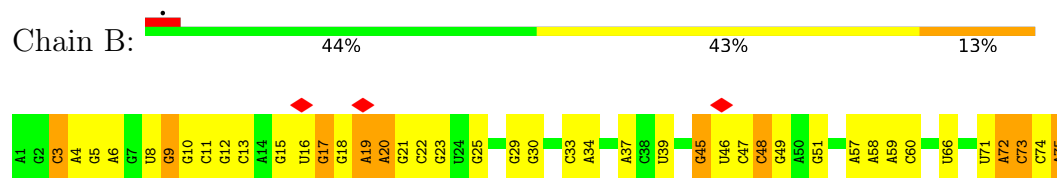
- Molecule 79: 60S ribosomal protein L23



- Molecule 80: 60S ribosomal protein L14



- Molecule 81: P-tRNA

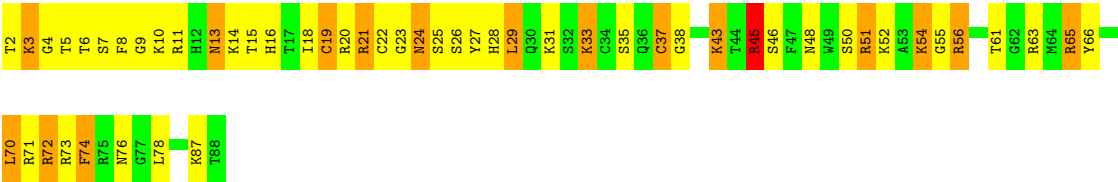


- Molecule 82: mRNA



- Molecule 83: Probable 60S ribosomal protein L37-B

Chain Cj:  39% 41% 18% .



## 4 Experimental information

| Property                             | Value                           | Source    |
|--------------------------------------|---------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                 | Depositor |
| Imposed symmetry                     | POINT, C1                       | Depositor |
| Number of particles used             | 10392                           | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF               | Depositor |
| CTF correction method                | PHASE FLIPPING ONLY             | Depositor |
| Microscope                           | FEI TITAN KRIOS                 | Depositor |
| Voltage (kV)                         | 300                             | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 80                              | Depositor |
| Minimum defocus (nm)                 | Not provided                    |           |
| Maximum defocus (nm)                 | Not provided                    |           |
| Magnification                        | Not provided                    |           |
| Image detector                       | FEI FALCON II (4k x 4k)         | Depositor |
| Maximum map value                    | 0.643                           | Depositor |
| Minimum map value                    | -0.491                          | Depositor |
| Average map value                    | 0.001                           | Depositor |
| Map value standard deviation         | 0.020                           | Depositor |
| Recommended contour level            | 0.035                           | Depositor |
| Map size ( $\text{\AA}$ )            | 426.00003, 426.00003, 426.00003 | wwPDB     |
| Map dimensions                       | 400, 400, 400                   | wwPDB     |
| Map angles ( $^\circ$ )              | 90.0, 90.0, 90.0                | wwPDB     |
| Pixel spacing ( $\text{\AA}$ )       | 1.065, 1.065, 1.065             | Depositor |

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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   | AA    | 0.28         | 0/1777        | 0.67        | 0/2422         |
| 2   | CA    | 0.74         | 1/1970 (0.1%) | 0.93        | 1/2635 (0.0%)  |
| 3   | AB    | 0.26         | 0/1825        | 0.65        | 0/2448         |
| 4   | CB    | 0.70         | 5/3356 (0.1%) | 0.97        | 7/4494 (0.2%)  |
| 5   | AC    | 0.31         | 0/1785        | 0.72        | 3/2415 (0.1%)  |
| 6   | CC    | 0.68         | 1/3163 (0.0%) | 0.95        | 10/4253 (0.2%) |
| 7   | Ag    | 0.21         | 0/2574        | 0.52        | 0/3506         |
| 8   | AU    | 0.26         | 0/825         | 0.57        | 0/1111         |
| 9   | AO    | 0.36         | 0/1016        | 0.84        | 4/1364 (0.3%)  |
| 10  | AX    | 0.38         | 0/1152        | 0.74        | 0/1540         |
| 11  | AM    | 0.25         | 0/937         | 0.68        | 2/1260 (0.2%)  |
| 12  | AS    | 0.25         | 0/1146        | 0.70        | 3/1535 (0.2%)  |
| 13  | Ad    | 0.30         | 0/443         | 0.77        | 0/589          |
| 14  | AN    | 0.34         | 0/1225        | 0.68        | 2/1641 (0.1%)  |
| 15  | AL    | 0.32         | 0/1296        | 0.65        | 0/1725         |
| 16  | AR    | 0.26         | 0/993         | 0.67        | 2/1333 (0.2%)  |
| 17  | AP    | 0.27         | 0/1036        | 0.66        | 0/1383         |
| 18  | AV    | 0.28         | 0/622         | 0.62        | 0/835          |
| 19  | AY    | 0.28         | 0/1032        | 0.70        | 2/1373 (0.1%)  |
| 20  | AZ    | 0.24         | 0/616         | 0.62        | 0/826          |
| 21  | Aa    | 0.40         | 0/883         | 0.88        | 4/1184 (0.3%)  |
| 22  | Ab    | 0.22         | 0/668         | 0.60        | 0/898          |
| 23  | AD    | 0.30         | 1/1808 (0.1%) | 0.65        | 0/2427         |
| 24  | Ae    | 0.30         | 0/475         | 0.85        | 2/625 (0.3%)   |
| 25  | Af    | 0.25         | 0/672         | 0.76        | 4/887 (0.5%)   |
| 26  | AJ    | 0.27         | 0/1526        | 0.70        | 2/2037 (0.1%)  |
| 27  | Ca    | 0.73         | 0/1235        | 1.00        | 5/1640 (0.3%)  |
| 28  | CN    | 0.85         | 0/1750        | 1.04        | 0/2335         |
| 29  | CI    | 0.34         | 0/1827        | 0.77        | 4/2447 (0.2%)  |
| 30  | CD    | 0.33         | 0/2379        | 0.68        | 4/3196 (0.1%)  |
| 31  | CQ    | 0.63         | 1/1544 (0.1%) | 0.89        | 3/2069 (0.1%)  |
| 32  | CR    | 0.45         | 0/1703        | 0.69        | 1/2255 (0.0%)  |
| 33  | CS    | 0.51         | 0/1491        | 0.92        | 1/1998 (0.1%)  |
| 34  | CT    | 0.57         | 1/1326 (0.1%) | 1.00        | 8/1773 (0.5%)  |

| Mol | Chain | Bond lengths |                | Bond angles |                  |
|-----|-------|--------------|----------------|-------------|------------------|
|     |       | RMSZ         | # Z  >5        | RMSZ        | # Z  >5          |
| 35  | CP    | 0.72         | 0/1529         | 0.89        | 1/2042 (0.0%)    |
| 36  | CX    | 0.42         | 0/1001         | 0.80        | 5/1348 (0.4%)    |
| 37  | CY    | 0.48         | 0/1094         | 0.71        | 0/1456           |
| 38  | CZ    | 0.31         | 0/1141         | 0.58        | 0/1517           |
| 39  | Cr    | 0.57         | 1/1069 (0.1%)  | 1.15        | 8/1432 (0.6%)    |
| 40  | Ch    | 0.38         | 0/1024         | 0.71        | 0/1353           |
| 41  | Cb    | 0.53         | 0/628          | 1.11        | 6/832 (0.7%)     |
| 42  | Cc    | 0.34         | 0/779          | 0.63        | 1/1048 (0.1%)    |
| 43  | Cd    | 0.66         | 0/939          | 0.87        | 0/1262           |
| 44  | Ce    | 0.86         | 0/1132         | 1.11        | 3/1508 (0.2%)    |
| 45  | Cf    | 0.62         | 0/1270         | 1.00        | 4/1696 (0.2%)    |
| 46  | Ci    | 0.37         | 0/944          | 0.86        | 2/1250 (0.2%)    |
| 47  | Ck    | 0.30         | 0/583          | 0.70        | 2/774 (0.3%)     |
| 48  | Cl    | 0.78         | 0/445          | 1.06        | 1/589 (0.2%)     |
| 49  | Cm    | 0.34         | 0/435          | 0.65        | 0/575            |
| 50  | Cn    | 0.61         | 0/237          | 0.80        | 0/300            |
| 51  | Cp    | 0.63         | 0/719          | 0.87        | 0/954            |
| 52  | Co    | 0.47         | 0/887          | 0.81        | 1/1162 (0.1%)    |
| 53  | CJ    | 0.26         | 0/1494         | 0.72        | 3/2001 (0.1%)    |
| 54  | CH    | 0.34         | 0/1519         | 0.72        | 4/2042 (0.2%)    |
| 55  | CE    | 0.35         | 0/1883         | 0.86        | 8/2514 (0.3%)    |
| 56  | CG    | 0.34         | 0/1968         | 0.75        | 4/2637 (0.2%)    |
| 57  | A9    | 0.51         | 0/714          | 0.63        | 0/1112           |
| 58  | A7    | 0.48         | 0/2854         | 0.49        | 0/4447           |
| 59  | A8    | 0.75         | 0/2932         | 0.82        | 2/4568 (0.0%)    |
| 60  | Cz    | 0.25         | 0/1727         | 0.66        | 0/2308           |
| 61  | B2    | 0.57         | 6/43887 (0.0%) | 0.47        | 3/68161 (0.0%)   |
| 62  | A5    | 0.75         | 2/86239 (0.0%) | 0.76        | 20/134149 (0.0%) |
| 63  | Ac    | 0.23         | 0/502          | 0.66        | 1/670 (0.1%)     |
| 64  | AW    | 0.35         | 1/1046 (0.1%)  | 0.65        | 1/1402 (0.1%)    |
| 65  | CW    | 0.55         | 0/495          | 0.81        | 2/658 (0.3%)     |
| 66  | Cg    | 0.57         | 0/863          | 0.95        | 2/1152 (0.2%)    |
| 67  | CU    | 0.27         | 0/828          | 0.62        | 0/1110           |
| 68  | AK    | 0.31         | 0/786          | 0.74        | 2/1064 (0.2%)    |
| 69  | AT    | 0.34         | 0/1060         | 0.90        | 8/1421 (0.6%)    |
| 70  | AF    | 2.71         | 2/1510 (0.1%)  | 0.80        | 4/2026 (0.2%)    |
| 71  | CF    | 0.66         | 0/1931         | 0.96        | 1/2587 (0.0%)    |
| 72  | AE    | 0.24         | 0/2096         | 0.60        | 0/2819           |
| 73  | AG    | 0.21         | 0/1891         | 0.54        | 0/2519           |
| 74  | AH    | 0.28         | 0/1593         | 0.70        | 1/2145 (0.0%)    |
| 75  | AI    | 0.32         | 0/1689         | 0.80        | 5/2250 (0.2%)    |
| 76  | AQ    | 0.30         | 0/1202         | 0.79        | 4/1608 (0.2%)    |
| 77  | CO    | 0.64         | 0/1700         | 0.93        | 2/2277 (0.1%)    |

| Mol | Chain | Bond lengths |                  | Bond angles |                   |
|-----|-------|--------------|------------------|-------------|-------------------|
|     |       | RMSZ         | # Z  >5          | RMSZ        | # Z  >5           |
| 78  | CL    | 0.55         | 0/1726           | 1.08        | 6/2308 (0.3%)     |
| 79  | CV    | 0.59         | 0/1014           | 0.82        | 0/1362            |
| 80  | CM    | 0.37         | 0/1326           | 0.77        | 4/1780 (0.2%)     |
| 81  | B     | 0.28         | 0/1796           | 0.49        | 0/2800            |
| 82  | v     | 0.29         | 0/283            | 0.47        | 0/439             |
| 83  | Cj    | 0.85         | 0/707            | 1.11        | 1/932 (0.1%)      |
| All | All   | 0.64         | 22/235193 (0.0%) | 0.72        | 196/344825 (0.1%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 2   | CA    | 0                   | 9                   |
| 3   | AB    | 0                   | 2                   |
| 4   | CB    | 0                   | 9                   |
| 5   | AC    | 0                   | 1                   |
| 6   | CC    | 0                   | 6                   |
| 8   | AU    | 0                   | 1                   |
| 10  | AX    | 0                   | 2                   |
| 12  | AS    | 0                   | 1                   |
| 13  | Ad    | 0                   | 2                   |
| 21  | Aa    | 0                   | 3                   |
| 23  | AD    | 0                   | 2                   |
| 24  | Ae    | 0                   | 2                   |
| 26  | AJ    | 0                   | 2                   |
| 27  | Ca    | 0                   | 8                   |
| 28  | CN    | 0                   | 11                  |
| 29  | CI    | 0                   | 2                   |
| 30  | CD    | 0                   | 4                   |
| 31  | CQ    | 0                   | 5                   |
| 32  | CR    | 0                   | 5                   |
| 33  | CS    | 0                   | 10                  |
| 34  | CT    | 0                   | 5                   |
| 35  | CP    | 0                   | 6                   |
| 39  | Cr    | 0                   | 11                  |
| 41  | Cb    | 0                   | 5                   |
| 43  | Cd    | 0                   | 4                   |
| 44  | Ce    | 0                   | 7                   |
| 45  | Cf    | 0                   | 4                   |
| 46  | Ci    | 0                   | 4                   |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 47  | Ck    | 0                   | 1                   |
| 48  | Cl    | 0                   | 3                   |
| 50  | Cn    | 0                   | 1                   |
| 51  | Cp    | 0                   | 1                   |
| 52  | Co    | 0                   | 3                   |
| 53  | CJ    | 0                   | 1                   |
| 55  | CE    | 0                   | 7                   |
| 56  | CG    | 0                   | 7                   |
| 63  | Ac    | 0                   | 1                   |
| 65  | CW    | 0                   | 2                   |
| 66  | Cg    | 0                   | 2                   |
| 69  | AT    | 0                   | 3                   |
| 70  | AF    | 0                   | 1                   |
| 71  | CF    | 0                   | 3                   |
| 72  | AE    | 0                   | 2                   |
| 73  | AG    | 0                   | 1                   |
| 74  | AH    | 0                   | 3                   |
| 75  | AI    | 0                   | 1                   |
| 77  | CO    | 0                   | 8                   |
| 78  | CL    | 0                   | 9                   |
| 80  | CM    | 0                   | 1                   |
| All | All   | 0                   | 194                 |

All (22) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms  | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|--------|-------------|----------|
| 70  | AF    | 190  | ILE  | CB-CG1 | 104.44 | 3.62        | 1.53     |
| 61  | B2    | 1727 | U    | N1-C2  | 40.97  | 2.20        | 1.38     |
| 61  | B2    | 1727 | U    | N3-C4  | 40.84  | 2.20        | 1.38     |
| 61  | B2    | 1727 | U    | C2-N3  | 40.45  | 2.18        | 1.37     |
| 61  | B2    | 1727 | U    | N1-C6  | 38.02  | 2.13        | 1.38     |
| 61  | B2    | 1727 | U    | C4-C5  | 36.44  | 2.16        | 1.43     |
| 61  | B2    | 1727 | U    | C5-C6  | 32.60  | 1.99        | 1.34     |
| 4   | CB    | 17   | TYR  | C-N    | -10.93 | 1.25        | 1.33     |
| 2   | CA    | 194  | ASN  | CA-CB  | -6.88  | 1.32        | 1.53     |
| 23  | AD    | 204  | LYS  | C-O    | -6.37  | 1.20        | 1.23     |
| 6   | CC    | 132  | ALA  | CA-C   | -6.26  | 1.41        | 1.52     |
| 70  | AF    | 190  | ILE  | CB-CG2 | 6.13   | 1.72        | 1.52     |
| 4   | CB    | 243  | LYS  | CA-C   | -6.12  | 1.44        | 1.52     |
| 39  | Cr    | 128  | ALA  | C-N    | 5.69   | 1.38        | 1.33     |
| 34  | CT    | 52   | LEU  | C-N    | -5.50  | 1.27        | 1.33     |
| 4   | CB    | 242  | ARG  | C-N    | -5.38  | 1.26        | 1.33     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 64  | AW    | 93   | LEU  | C-N   | -5.29 | 1.24        | 1.33     |
| 4   | CB    | 18   | PRO  | N-CA  | -5.24 | 1.44        | 1.47     |
| 62  | A5    | 1674 | A    | C5-C6 | -5.19 | 1.30        | 1.41     |
| 62  | A5    | 2529 | G    | C5-C6 | -5.08 | 1.32        | 1.42     |
| 31  | CQ    | 174  | PHE  | CB-CG | -5.02 | 1.39        | 1.50     |
| 4   | CB    | 257  | TRP  | C-N   | -5.02 | 1.23        | 1.33     |

All (196) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms      | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 29  | CI    | 91  | LEU  | CA-C-N     | 13.65  | 140.59      | 121.61   |
| 29  | CI    | 91  | LEU  | C-N-CA     | 13.65  | 140.59      | 121.61   |
| 70  | AF    | 190 | ILE  | CA-CB-CG1  | 11.76  | 130.39      | 110.40   |
| 59  | A8    | 100 | G    | OP1-P-O3'  | -10.73 | 75.80       | 108.00   |
| 70  | AF    | 190 | ILE  | CB-CG1-CD1 | 10.00  | 134.79      | 113.80   |
| 69  | AT    | 47  | PRO  | CA-N-CD    | -9.22  | 99.09       | 112.00   |
| 70  | AF    | 190 | ILE  | CA-CB-CG2  | -9.17  | 94.90       | 110.50   |
| 69  | AT    | 31  | PRO  | CA-N-CD    | -9.13  | 99.22       | 112.00   |
| 69  | AT    | 50  | PRO  | CA-N-CD    | -9.12  | 99.23       | 112.00   |
| 34  | CT    | 144 | LEU  | CA-C-N     | 8.99   | 137.89      | 121.70   |
| 34  | CT    | 144 | LEU  | C-N-CA     | 8.99   | 137.89      | 121.70   |
| 69  | AT    | 69  | PRO  | CA-N-CD    | -8.64  | 99.90       | 112.00   |
| 69  | AT    | 89  | PRO  | CA-N-CD    | -8.37  | 99.78       | 111.50   |
| 77  | CO    | 48  | HIS  | N-CA-C     | 7.96   | 118.48      | 108.45   |
| 68  | AK    | 54  | GLY  | CA-C-N     | 7.90   | 135.91      | 121.70   |
| 68  | AK    | 54  | GLY  | C-N-CA     | 7.90   | 135.91      | 121.70   |
| 5   | AC    | 242 | MET  | N-CA-C     | 7.86   | 115.20      | 108.13   |
| 4   | CB    | 55  | HIS  | N-CA-C     | 7.83   | 120.07      | 110.91   |
| 26  | AJ    | 5   | ARG  | CA-C-N     | 7.70   | 135.56      | 121.70   |
| 26  | AJ    | 5   | ARG  | C-N-CA     | 7.70   | 135.56      | 121.70   |
| 6   | CC    | 35  | ILE  | CA-C-N     | -7.64  | 108.76      | 122.28   |
| 6   | CC    | 35  | ILE  | C-N-CA     | -7.64  | 108.76      | 122.28   |
| 6   | CC    | 195 | GLY  | CA-C-N     | 7.50   | 135.19      | 121.70   |
| 6   | CC    | 195 | GLY  | C-N-CA     | 7.50   | 135.19      | 121.70   |
| 11  | AM    | 39  | VAL  | CA-C-N     | 7.47   | 135.15      | 121.70   |
| 11  | AM    | 39  | VAL  | C-N-CA     | 7.47   | 135.15      | 121.70   |
| 59  | A8    | 100 | G    | OP2-P-O3'  | -7.46  | 85.61       | 108.00   |
| 4   | CB    | 4   | ARG  | CA-C-N     | 7.34   | 135.56      | 121.54   |
| 4   | CB    | 4   | ARG  | C-N-CA     | 7.34   | 135.56      | 121.54   |
| 30  | CD    | 188 | LYS  | CA-C-N     | 7.32   | 134.88      | 121.70   |
| 30  | CD    | 188 | LYS  | C-N-CA     | 7.32   | 134.88      | 121.70   |
| 24  | Ae    | 116 | ASN  | CA-C-N     | 7.27   | 134.79      | 121.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 24  | Ae    | 116  | ASN  | C-N-CA     | 7.27  | 134.79      | 121.70   |
| 71  | CF    | 237  | PHE  | N-CA-C     | 7.26  | 126.26      | 110.80   |
| 70  | AF    | 190  | ILE  | CG1-CB-CG2 | 7.08  | 131.93      | 110.70   |
| 62  | A5    | 1784 | A    | P-O3'-C3'  | 6.99  | 130.68      | 120.20   |
| 27  | Ca    | 98   | LYS  | CA-C-N     | 6.96  | 134.23      | 121.70   |
| 27  | Ca    | 98   | LYS  | C-N-CA     | 6.96  | 134.23      | 121.70   |
| 41  | Cb    | 25   | LEU  | N-CA-C     | -6.96 | 98.63       | 108.23   |
| 34  | CT    | 144  | LEU  | N-CA-C     | 6.95  | 127.66      | 113.20   |
| 42  | Cc    | 104  | ILE  | N-CA-C     | -6.93 | 105.97      | 112.83   |
| 41  | Cb    | 38   | LYS  | CA-C-N     | 6.87  | 134.06      | 121.70   |
| 41  | Cb    | 38   | LYS  | C-N-CA     | 6.87  | 134.06      | 121.70   |
| 34  | CT    | 6    | GLY  | N-CA-C     | 6.83  | 133.10      | 113.30   |
| 41  | Cb    | 39   | PHE  | N-CA-C     | 6.75  | 129.89      | 111.00   |
| 54  | CH    | 106  | ASN  | CA-C-N     | 6.65  | 133.67      | 121.70   |
| 54  | CH    | 106  | ASN  | C-N-CA     | 6.65  | 133.67      | 121.70   |
| 44  | Ce    | 128  | LEU  | CA-C-N     | 6.58  | 133.53      | 121.70   |
| 44  | Ce    | 128  | LEU  | C-N-CA     | 6.58  | 133.53      | 121.70   |
| 80  | CM    | 134  | THR  | CA-C-N     | 6.58  | 133.53      | 121.70   |
| 80  | CM    | 134  | THR  | C-N-CA     | 6.58  | 133.53      | 121.70   |
| 34  | CT    | 149  | ALA  | CA-C-N     | 6.54  | 133.47      | 121.70   |
| 34  | CT    | 149  | ALA  | C-N-CA     | 6.54  | 133.47      | 121.70   |
| 80  | CM    | 153  | ALA  | CA-C-N     | 6.51  | 133.42      | 121.70   |
| 80  | CM    | 153  | ALA  | C-N-CA     | 6.51  | 133.42      | 121.70   |
| 6   | CC    | 364  | GLU  | CA-C-N     | 6.50  | 133.40      | 121.70   |
| 6   | CC    | 364  | GLU  | C-N-CA     | 6.50  | 133.40      | 121.70   |
| 45  | Cf    | 16   | LYS  | CA-C-N     | 6.42  | 133.25      | 121.70   |
| 45  | Cf    | 16   | LYS  | C-N-CA     | 6.42  | 133.25      | 121.70   |
| 63  | Ac    | 18   | GLY  | N-CA-C     | 6.42  | 120.25      | 112.49   |
| 5   | AC    | 39   | ASP  | CA-C-N     | 6.41  | 133.24      | 121.70   |
| 5   | AC    | 39   | ASP  | C-N-CA     | 6.41  | 133.24      | 121.70   |
| 4   | CB    | 324  | GLY  | N-CA-C     | 6.40  | 128.35      | 113.18   |
| 62  | A5    | 1080 | G    | C8-N9-C1'  | -6.28 | 108.15      | 127.00   |
| 78  | CL    | 162  | ALA  | CA-C-N     | 6.23  | 132.91      | 121.70   |
| 78  | CL    | 162  | ALA  | C-N-CA     | 6.23  | 132.91      | 121.70   |
| 55  | CE    | 65   | SER  | CA-C-N     | 6.22  | 132.90      | 121.70   |
| 55  | CE    | 65   | SER  | C-N-CA     | 6.22  | 132.90      | 121.70   |
| 2   | CA    | 248  | GLY  | N-CA-C     | 6.22  | 118.97      | 110.58   |
| 35  | CP    | 66   | GLY  | N-CA-C     | 6.21  | 131.31      | 113.30   |
| 78  | CL    | 163  | VAL  | CA-C-N     | 6.20  | 132.86      | 121.70   |
| 78  | CL    | 163  | VAL  | C-N-CA     | 6.20  | 132.86      | 121.70   |
| 76  | AQ    | 3    | GLN  | CA-C-N     | 6.20  | 132.85      | 121.70   |
| 76  | AQ    | 3    | GLN  | C-N-CA     | 6.20  | 132.85      | 121.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 9   | AO    | 99   | ALA  | CA-C-N      | 6.18  | 132.82      | 121.70   |
| 9   | AO    | 99   | ALA  | C-N-CA      | 6.18  | 132.82      | 121.70   |
| 62  | A5    | 1080 | G    | C4-N9-C1'   | 6.18  | 145.03      | 126.50   |
| 62  | A5    | 3326 | G    | N9-C1'-C2'  | 6.14  | 123.20      | 114.00   |
| 31  | CQ    | 116  | ALA  | CA-C-N      | 6.11  | 132.69      | 121.70   |
| 31  | CQ    | 116  | ALA  | C-N-CA      | 6.11  | 132.69      | 121.70   |
| 21  | Aa    | 63   | VAL  | CA-C-N      | 6.09  | 128.83      | 120.67   |
| 21  | Aa    | 63   | VAL  | C-N-CA      | 6.09  | 128.83      | 120.67   |
| 33  | CS    | 54   | PHE  | N-CA-C      | 6.08  | 118.62      | 111.02   |
| 44  | Ce    | 52   | TYR  | CA-CB-CG    | 6.07  | 124.82      | 113.90   |
| 36  | CX    | 186  | VAL  | CA-C-N      | 6.06  | 141.55      | 127.00   |
| 36  | CX    | 186  | VAL  | C-N-CA      | 6.06  | 141.55      | 127.00   |
| 25  | Af    | 88   | PRO  | CA-C-N      | 6.04  | 133.07      | 121.54   |
| 25  | Af    | 88   | PRO  | C-N-CA      | 6.04  | 133.07      | 121.54   |
| 39  | Cr    | 35   | ASN  | CA-C-N      | 5.97  | 132.95      | 121.54   |
| 39  | Cr    | 35   | ASN  | C-N-CA      | 5.97  | 132.95      | 121.54   |
| 74  | AH    | 112  | GLN  | CA-CB-CG    | 5.96  | 126.02      | 114.10   |
| 75  | AI    | 19   | LYS  | CA-C-N      | -5.92 | 114.44      | 121.90   |
| 75  | AI    | 19   | LYS  | C-N-CA      | -5.92 | 114.44      | 121.90   |
| 14  | AN    | 58   | HIS  | CA-C-N      | 5.92  | 132.35      | 121.70   |
| 14  | AN    | 58   | HIS  | C-N-CA      | 5.92  | 132.35      | 121.70   |
| 62  | A5    | 3396 | A    | C2'-C3'-O3' | 5.88  | 122.53      | 113.70   |
| 53  | CJ    | 102  | GLU  | CA-C-N      | 5.88  | 132.28      | 121.70   |
| 53  | CJ    | 102  | GLU  | C-N-CA      | 5.88  | 132.28      | 121.70   |
| 39  | Cr    | 42   | TYR  | N-CA-C      | -5.87 | 103.54      | 112.99   |
| 65  | CW    | 25   | ASP  | CA-C-N      | 5.87  | 132.26      | 121.70   |
| 65  | CW    | 25   | ASP  | C-N-CA      | 5.87  | 132.26      | 121.70   |
| 9   | AO    | 105  | THR  | N-CA-C      | 5.84  | 118.40      | 111.33   |
| 29  | CI    | 109  | ASP  | CA-C-N      | 5.82  | 130.66      | 122.46   |
| 29  | CI    | 109  | ASP  | C-N-CA      | 5.82  | 130.66      | 122.46   |
| 21  | Aa    | 107  | ALA  | CA-C-N      | 5.81  | 132.16      | 121.70   |
| 21  | Aa    | 107  | ALA  | C-N-CA      | 5.81  | 132.16      | 121.70   |
| 25  | Af    | 151  | SER  | CA-C-N      | 5.80  | 132.14      | 121.70   |
| 25  | Af    | 151  | SER  | C-N-CA      | 5.80  | 132.14      | 121.70   |
| 62  | A5    | 2739 | A    | C4-N9-C1'   | 5.79  | 143.67      | 126.30   |
| 45  | Cf    | 138  | ASN  | N-CA-C      | 5.78  | 123.11      | 110.80   |
| 75  | AI    | 22   | ARG  | CA-CB-CG    | 5.76  | 125.63      | 114.10   |
| 66  | Cg    | 34   | TYR  | CA-CB-CG    | 5.75  | 124.25      | 113.90   |
| 27  | Ca    | 93   | LYS  | CA-C-N      | 5.70  | 131.97      | 121.70   |
| 27  | Ca    | 93   | LYS  | C-N-CA      | 5.70  | 131.97      | 121.70   |
| 76  | AQ    | 117  | TYR  | CA-C-N      | 5.70  | 132.43      | 121.54   |
| 76  | AQ    | 117  | TYR  | C-N-CA      | 5.70  | 132.43      | 121.54   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 27  | Ca    | 37   | GLY  | N-CA-C      | -5.68 | 96.84       | 113.30   |
| 83  | Cj    | 23   | GLY  | N-CA-C      | -5.62 | 107.56      | 113.58   |
| 55  | CE    | 193  | VAL  | CA-C-N      | 5.58  | 140.39      | 127.00   |
| 55  | CE    | 193  | VAL  | C-N-CA      | 5.58  | 140.39      | 127.00   |
| 30  | CD    | 267  | ARG  | CA-C-N      | 5.57  | 131.72      | 121.70   |
| 30  | CD    | 267  | ARG  | C-N-CA      | 5.57  | 131.72      | 121.70   |
| 78  | CL    | 169  | VAL  | CA-C-N      | 5.55  | 131.69      | 121.70   |
| 78  | CL    | 169  | VAL  | C-N-CA      | 5.55  | 131.69      | 121.70   |
| 46  | Ci    | 31   | VAL  | CA-C-N      | 5.53  | 131.66      | 121.70   |
| 46  | Ci    | 31   | VAL  | C-N-CA      | 5.53  | 131.66      | 121.70   |
| 61  | B2    | 1949 | A    | P-O3'-C3'   | 5.51  | 128.47      | 120.20   |
| 6   | CC    | 314  | ARG  | CA-C-N      | 5.51  | 130.23      | 122.46   |
| 6   | CC    | 314  | ARG  | C-N-CA      | 5.51  | 130.23      | 122.46   |
| 45  | Cf    | 46   | ARG  | CA-CB-CG    | 5.50  | 125.10      | 114.10   |
| 62  | A5    | 1784 | A    | C4'-C3'-O3' | 5.48  | 117.63      | 109.40   |
| 4   | CB    | 245  | HIS  | N-CA-CB     | -5.47 | 100.97      | 109.34   |
| 6   | CC    | 297  | LYS  | CA-C-N      | 5.46  | 131.54      | 121.70   |
| 6   | CC    | 297  | LYS  | C-N-CA      | 5.46  | 131.54      | 121.70   |
| 12  | AS    | 89   | ASP  | CA-C-N      | 5.44  | 131.49      | 121.70   |
| 12  | AS    | 89   | ASP  | C-N-CA      | 5.44  | 131.49      | 121.70   |
| 61  | B2    | 1849 | U    | P-O3'-C3'   | 5.43  | 128.35      | 120.20   |
| 62  | A5    | 374  | C    | C2-N1-C1'   | 5.43  | 135.08      | 118.80   |
| 19  | AY    | 103  | GLN  | CA-C-N      | 5.43  | 131.47      | 121.70   |
| 19  | AY    | 103  | GLN  | C-N-CA      | 5.43  | 131.47      | 121.70   |
| 55  | CE    | 26   | LEU  | CA-C-N      | 5.41  | 131.43      | 121.70   |
| 55  | CE    | 26   | LEU  | C-N-CA      | 5.41  | 131.43      | 121.70   |
| 62  | A5    | 1620 | A    | C4-N9-C1'   | 5.40  | 142.50      | 126.30   |
| 62  | A5    | 429  | U    | N1-C1'-C2'  | 5.39  | 120.09      | 112.00   |
| 39  | Cr    | 72   | LYS  | CA-C-N      | 5.39  | 131.83      | 121.54   |
| 39  | Cr    | 72   | LYS  | C-N-CA      | 5.39  | 131.83      | 121.54   |
| 62  | A5    | 2162 | C    | C2-N1-C1'   | 5.37  | 134.91      | 118.80   |
| 4   | CB    | 2    | SER  | CA-C-N      | 5.36  | 131.78      | 121.54   |
| 4   | CB    | 2    | SER  | C-N-CA      | 5.36  | 131.78      | 121.54   |
| 62  | A5    | 1719 | G    | C4-N9-C1'   | 5.36  | 142.58      | 126.50   |
| 31  | CQ    | 163  | THR  | N-CA-C      | 5.36  | 119.05      | 112.03   |
| 55  | CE    | 174  | LYS  | CA-C-N      | 5.35  | 131.77      | 121.54   |
| 55  | CE    | 174  | LYS  | C-N-CA      | 5.35  | 131.77      | 121.54   |
| 34  | CT    | 145  | GLU  | N-CA-C      | 5.33  | 125.93      | 111.00   |
| 62  | A5    | 2129 | C    | P-O3'-C3'   | 5.33  | 128.20      | 120.20   |
| 64  | AW    | 28   | ARG  | C-N-CD      | -5.33 | 108.88      | 120.60   |
| 62  | A5    | 1646 | U    | N1-C1'-C2'  | 5.32  | 119.98      | 112.00   |
| 16  | AR    | 94   | ASP  | CA-C-N      | 5.32  | 131.27      | 121.70   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 16  | AR    | 94   | ASP  | C-N-CA      | 5.32  | 131.27      | 121.70   |
| 66  | Cg    | 79   | VAL  | N-CA-C      | -5.28 | 107.24      | 113.42   |
| 32  | CR    | 166  | VAL  | N-CA-C      | -5.28 | 107.21      | 111.91   |
| 56  | CG    | 204  | CYS  | CA-C-N      | 5.26  | 131.59      | 121.54   |
| 56  | CG    | 204  | CYS  | C-N-CA      | 5.26  | 131.59      | 121.54   |
| 69  | AT    | 147  | LYS  | CA-C-N      | -5.26 | 112.23      | 121.70   |
| 69  | AT    | 147  | LYS  | C-N-CA      | -5.26 | 112.23      | 121.70   |
| 62  | A5    | 3677 | U    | O5'-C5'-C4' | 5.25  | 119.58      | 111.70   |
| 47  | Ck    | 58   | GLN  | CA-C-N      | 5.25  | 131.15      | 121.70   |
| 47  | Ck    | 58   | GLN  | C-N-CA      | 5.25  | 131.15      | 121.70   |
| 62  | A5    | 1614 | A    | C8-N9-C1'   | -5.25 | 111.96      | 127.70   |
| 77  | CO    | 113  | PRO  | N-CA-C      | 5.25  | 123.28      | 112.47   |
| 39  | Cr    | 58   | ALA  | CA-C-N      | 5.21  | 131.08      | 121.70   |
| 39  | Cr    | 58   | ALA  | C-N-CA      | 5.21  | 131.08      | 121.70   |
| 62  | A5    | 1104 | A    | C4-N9-C1'   | 5.21  | 141.92      | 126.30   |
| 62  | A5    | 3676 | C    | C4'-C3'-O3' | 5.19  | 120.79      | 113.00   |
| 34  | CT    | 144  | LEU  | CA-CB-CG    | 5.19  | 134.45      | 116.30   |
| 56  | CG    | 41   | PRO  | CA-C-N      | 5.18  | 131.02      | 121.70   |
| 56  | CG    | 41   | PRO  | C-N-CA      | 5.18  | 131.02      | 121.70   |
| 61  | B2    | 1765 | U    | P-O3'-C3'   | 5.17  | 127.96      | 120.20   |
| 48  | Cl    | 37   | TYR  | CA-CB-CG    | 5.17  | 123.21      | 113.90   |
| 62  | A5    | 1358 | U    | O5'-P-OP1   | -5.15 | 92.56       | 108.00   |
| 53  | CJ    | 10   | ARG  | N-CA-C      | -5.13 | 107.69      | 114.31   |
| 41  | Cb    | 10   | HIS  | CA-C-N      | 5.12  | 131.32      | 121.54   |
| 41  | Cb    | 10   | HIS  | C-N-CA      | 5.12  | 131.32      | 121.54   |
| 52  | Co    | 47   | GLY  | N-CA-C      | 5.12  | 125.31      | 113.18   |
| 62  | A5    | 1801 | U    | O4'-C1'-N1  | 5.11  | 116.16      | 108.50   |
| 12  | AS    | 89   | ASP  | N-CA-C      | 5.10  | 119.73      | 111.37   |
| 9   | AO    | 146  | ARG  | CA-CB-CG    | 5.09  | 124.29      | 114.10   |
| 36  | CX    | 186  | VAL  | C-N-CD      | -5.08 | 109.42      | 120.60   |
| 36  | CX    | 179  | PRO  | CA-C-N      | 5.07  | 131.22      | 121.54   |
| 36  | CX    | 179  | PRO  | C-N-CA      | 5.07  | 131.22      | 121.54   |
| 54  | CH    | 21   | LYS  | CA-C-N      | 5.06  | 131.21      | 121.54   |
| 54  | CH    | 21   | LYS  | C-N-CA      | 5.06  | 131.21      | 121.54   |
| 75  | AI    | 141  | LYS  | CA-C-N      | 5.04  | 131.16      | 121.54   |
| 75  | AI    | 141  | LYS  | C-N-CA      | 5.04  | 131.16      | 121.54   |
| 69  | AT    | 42   | PHE  | N-CA-C      | -5.03 | 108.89      | 114.62   |
| 39  | Cr    | 48   | VAL  | N-CA-C      | -5.00 | 107.59      | 112.29   |

There are no chirality outliers.

All (194) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 3   | AB    | 118 | LYS  | Peptide |
| 3   | AB    | 119 | LYS  | Peptide |
| 5   | AC    | 241 | GLU  | Peptide |
| 23  | AD    | 195 | ASP  | Peptide |
| 23  | AD    | 202 | PRO  | Peptide |
| 72  | AE    | 240 | LYS  | Peptide |
| 72  | AE    | 241 | GLY  | Peptide |
| 70  | AF    | 190 | ILE  | Peptide |
| 73  | AG    | 99  | GLY  | Peptide |
| 74  | AH    | 100 | PRO  | Peptide |
| 74  | AH    | 187 | PHE  | Peptide |
| 74  | AH    | 64  | ILE  | Peptide |
| 75  | AI    | 98  | LYS  | Peptide |
| 26  | AJ    | 148 | PHE  | Peptide |
| 26  | AJ    | 149 | VAL  | Peptide |
| 12  | AS    | 88  | LYS  | Peptide |
| 69  | AT    | 82  | ARG  | Peptide |
| 69  | AT    | 86  | GLY  | Peptide |
| 69  | AT    | 88  | HIS  | Peptide |
| 8   | AU    | 76  | SER  | Peptide |
| 10  | AX    | 2   | GLY  | Peptide |
| 10  | AX    | 22  | TRP  | Peptide |
| 21  | Aa    | 10  | ARG  | Peptide |
| 21  | Aa    | 62  | TYR  | Peptide |
| 21  | Aa    | 85  | ARG  | Peptide |
| 63  | Ac    | 18  | GLY  | Peptide |
| 13  | Ad    | 33  | LYS  | Peptide |
| 13  | Ad    | 39  | CYS  | Peptide |
| 24  | Ae    | 116 | ASN  | Peptide |
| 24  | Ae    | 96  | LYS  | Peptide |
| 2   | CA    | 179 | ILE  | Peptide |
| 2   | CA    | 185 | ALA  | Peptide |
| 2   | CA    | 196 | TRP  | Peptide |
| 2   | CA    | 197 | PRO  | Peptide |
| 2   | CA    | 203 | ALA  | Peptide |
| 2   | CA    | 210 | PRO  | Peptide |
| 2   | CA    | 213 | GLY  | Peptide |
| 2   | CA    | 229 | THR  | Peptide |
| 2   | CA    | 3   | ARG  | Peptide |
| 4   | CB    | 16  | PHE  | Peptide |
| 4   | CB    | 17  | TYR  | Peptide |
| 4   | CB    | 234 | ARG  | Peptide |
| 4   | CB    | 244 | THR  | Peptide |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>Group</b> |
|------------|--------------|------------|-------------|--------------|
| 4          | CB           | 311        | ASP         | Peptide      |
| 4          | CB           | 323        | TYR         | Peptide      |
| 4          | CB           | 33         | PRO         | Peptide      |
| 4          | CB           | 333        | ILE         | Peptide      |
| 4          | CB           | 334        | LYS         | Peptide      |
| 6          | CC           | 315        | SER         | Peptide      |
| 6          | CC           | 60         | LEU         | Peptide      |
| 6          | CC           | 68         | GLU         | Peptide      |
| 6          | CC           | 82         | VAL         | Peptide      |
| 6          | CC           | 85         | GLY         | Peptide      |
| 6          | CC           | 92         | GLN         | Peptide      |
| 30         | CD           | 19         | LYS         | Peptide      |
| 30         | CD           | 222        | GLN         | Peptide      |
| 30         | CD           | 271        | LYS         | Peptide      |
| 30         | CD           | 272        | LYS         | Peptide      |
| 55         | CE           | 224        | LYS         | Peptide      |
| 55         | CE           | 228        | ASN         | Peptide      |
| 55         | CE           | 237        | TYR         | Peptide      |
| 55         | CE           | 60         | VAL         | Peptide      |
| 55         | CE           | 69         | TYR         | Peptide      |
| 55         | CE           | 70         | PRO         | Peptide      |
| 55         | CE           | 71         | THR         | Peptide      |
| 71         | CF           | 134        | ASN         | Peptide      |
| 71         | CF           | 209        | SER         | Peptide      |
| 71         | CF           | 235        | GLY         | Peptide      |
| 56         | CG           | 165        | ASP         | Peptide      |
| 56         | CG           | 168        | PRO         | Peptide      |
| 56         | CG           | 43         | ASN         | Peptide      |
| 56         | CG           | 83         | PRO         | Peptide      |
| 56         | CG           | 85         | ILE         | Peptide      |
| 56         | CG           | 86         | HIS         | Peptide      |
| 56         | CG           | 91         | THR         | Peptide      |
| 29         | CI           | 110        | ARG         | Peptide      |
| 29         | CI           | 111        | LEU         | Peptide      |
| 53         | CJ           | 96         | GLU         | Peptide      |
| 78         | CL           | 124        | ILE         | Peptide      |
| 78         | CL           | 152        | PRO         | Peptide      |
| 78         | CL           | 158        | ASN         | Peptide      |
| 78         | CL           | 160        | GLN         | Peptide      |
| 78         | CL           | 169        | VAL         | Peptide      |
| 78         | CL           | 46         | PHE         | Peptide      |
| 78         | CL           | 53         | ALA         | Peptide      |

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| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 78  | CL    | 75  | PHE  | Peptide |
| 78  | CL    | 97  | VAL  | Peptide |
| 80  | CM    | 103 | SER  | Peptide |
| 28  | CN    | 124 | ASP  | Peptide |
| 28  | CN    | 127 | TYR  | Peptide |
| 28  | CN    | 181 | SER  | Peptide |
| 28  | CN    | 182 | GLN  | Peptide |
| 28  | CN    | 190 | ALA  | Peptide |
| 28  | CN    | 192 | TRP  | Peptide |
| 28  | CN    | 28  | TRP  | Peptide |
| 28  | CN    | 47  | LYS  | Peptide |
| 28  | CN    | 76  | PRO  | Peptide |
| 28  | CN    | 78  | GLY  | Peptide |
| 28  | CN    | 79  | CYS  | Peptide |
| 77  | CO    | 111 | PRO  | Peptide |
| 77  | CO    | 112 | SER  | Peptide |
| 77  | CO    | 203 | TYR  | Peptide |
| 77  | CO    | 5   | THR  | Peptide |
| 77  | CO    | 52  | ASN  | Peptide |
| 77  | CO    | 59  | TYR  | Peptide |
| 77  | CO    | 64  | CYS  | Peptide |
| 77  | CO    | 71  | GLY  | Peptide |
| 35  | CP    | 125 | LEU  | Peptide |
| 35  | CP    | 27  | LYS  | Peptide |
| 35  | CP    | 63  | PHE  | Peptide |
| 35  | CP    | 68  | GLY  | Peptide |
| 35  | CP    | 69  | ARG  | Peptide |
| 35  | CP    | 78  | THR  | Peptide |
| 31  | CQ    | 155 | ALA  | Peptide |
| 31  | CQ    | 3   | ILE  | Peptide |
| 31  | CQ    | 4   | ASP  | Peptide |
| 31  | CQ    | 5   | ILE  | Peptide |
| 31  | CQ    | 58  | ARG  | Peptide |
| 32  | CR    | 112 | SER  | Peptide |
| 32  | CR    | 113 | LYS  | Peptide |
| 32  | CR    | 121 | HIS  | Peptide |
| 32  | CR    | 169 | ALA  | Peptide |
| 32  | CR    | 17  | CYS  | Peptide |
| 33  | CS    | 111 | ARG  | Peptide |
| 33  | CS    | 118 | ARG  | Peptide |
| 33  | CS    | 138 | ARG  | Peptide |
| 33  | CS    | 159 | HIS  | Peptide |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>Group</b> |
|------------|--------------|------------|-------------|--------------|
| 33         | CS           | 17         | LEU         | Peptide      |
| 33         | CS           | 170        | ARG         | Peptide      |
| 33         | CS           | 172        | PRO         | Peptide      |
| 33         | CS           | 53         | LYS         | Peptide      |
| 33         | CS           | 62         | VAL         | Peptide      |
| 33         | CS           | 67         | VAL         | Peptide      |
| 34         | CT           | 143        | LYS         | Peptide      |
| 34         | CT           | 145        | GLU         | Peptide      |
| 34         | CT           | 3          | ASN         | Peptide      |
| 34         | CT           | 4          | SER         | Peptide      |
| 34         | CT           | 6          | GLY         | Peptide      |
| 65         | CW           | 18         | GLY         | Peptide      |
| 65         | CW           | 38         | ARG         | Peptide      |
| 27         | Ca           | 14         | GLY         | Peptide      |
| 27         | Ca           | 27         | ARG         | Peptide      |
| 27         | Ca           | 3          | ASN         | Peptide      |
| 27         | Ca           | 45         | ASN         | Peptide      |
| 27         | Ca           | 56         | LYS         | Peptide      |
| 27         | Ca           | 58         | GLY         | Peptide      |
| 27         | Ca           | 80         | TRP         | Peptide      |
| 27         | Ca           | 98         | LYS         | Peptide      |
| 41         | Cb           | 21         | ILE         | Peptide      |
| 41         | Cb           | 23         | ARG         | Peptide      |
| 41         | Cb           | 25         | LEU         | Peptide      |
| 41         | Cb           | 35         | MET         | Peptide      |
| 41         | Cb           | 38         | LYS         | Peptide      |
| 43         | Cd           | 32         | ASN         | Peptide      |
| 43         | Cd           | 37         | LYS         | Peptide      |
| 43         | Cd           | 39         | ALA         | Peptide      |
| 43         | Cd           | 45         | GLU         | Peptide      |
| 44         | Ce           | 123        | ASN         | Peptide      |
| 44         | Ce           | 19         | PHE         | Peptide      |
| 44         | Ce           | 39         | GLY         | Peptide      |
| 44         | Ce           | 41         | ASP         | Peptide      |
| 44         | Ce           | 5          | PRO         | Peptide      |
| 44         | Ce           | 51         | GLN         | Peptide      |
| 44         | Ce           | 52         | TYR         | Peptide      |
| 45         | Cf           | 107        | HIS         | Peptide      |
| 45         | Cf           | 108        | PRO         | Peptide      |
| 45         | Cf           | 128        | THR         | Peptide      |
| 45         | Cf           | 37         | ALA         | Peptide      |
| 66         | Cg           | 18         | ASN         | Peptide      |

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| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 66  | Cg    | 50  | LYS  | Peptide |
| 46  | Ci    | 34  | LEU  | Peptide |
| 46  | Ci    | 61  | ALA  | Peptide |
| 46  | Ci    | 7   | LEU  | Peptide |
| 46  | Ci    | 87  | LEU  | Peptide |
| 47  | Ck    | 58  | GLN  | Peptide |
| 48  | Cl    | 37  | TYR  | Peptide |
| 48  | Cl    | 42  | ARG  | Peptide |
| 48  | Cl    | 7   | PHE  | Peptide |
| 50  | Cn    | 17  | ARG  | Peptide |
| 52  | Co    | 26  | TYR  | Peptide |
| 52  | Co    | 46  | GLN  | Peptide |
| 52  | Co    | 55  | ILE  | Peptide |
| 51  | Cp    | 7   | LYS  | Peptide |
| 39  | Cr    | 126 | LYS  | Peptide |
| 39  | Cr    | 26  | LYS  | Peptide |
| 39  | Cr    | 28  | PRO  | Peptide |
| 39  | Cr    | 37  | ALA  | Peptide |
| 39  | Cr    | 41  | SER  | Peptide |
| 39  | Cr    | 46  | GLY  | Peptide |
| 39  | Cr    | 69  | LYS  | Peptide |
| 39  | Cr    | 78  | ALA  | Peptide |
| 39  | Cr    | 79  | LYS  | Peptide |
| 39  | Cr    | 80  | ASN  | Peptide |
| 39  | Cr    | 81  | THR  | Peptide |

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | AA    | 1737  | 0        | 1750     | 59      | 0            |
| 2   | CA    | 1935  | 0        | 2037     | 91      | 0            |
| 3   | AB    | 1798  | 0        | 1867     | 58      | 0            |
| 4   | CB    | 3287  | 0        | 3432     | 110     | 0            |
| 5   | AC    | 1746  | 0        | 1827     | 61      | 0            |
| 6   | CC    | 3109  | 0        | 3298     | 125     | 0            |
| 7   | Ag    | 2511  | 0        | 2438     | 72      | 0            |
| 8   | AU    | 815   | 0        | 871      | 30      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 9   | AO    | 1003  | 0        | 1035     | 39      | 0            |
| 10  | AX    | 1131  | 0        | 1190     | 47      | 0            |
| 11  | AM    | 924   | 0        | 960      | 30      | 0            |
| 12  | AS    | 1128  | 0        | 1177     | 64      | 0            |
| 13  | Ad    | 433   | 0        | 424      | 19      | 0            |
| 14  | AN    | 1202  | 0        | 1291     | 38      | 0            |
| 15  | AL    | 1274  | 0        | 1351     | 40      | 0            |
| 16  | AR    | 981   | 0        | 1038     | 30      | 0            |
| 17  | AP    | 1016  | 0        | 1086     | 47      | 0            |
| 18  | AV    | 617   | 0        | 613      | 33      | 0            |
| 19  | AY    | 1016  | 0        | 1073     | 34      | 0            |
| 20  | AZ    | 608   | 0        | 658      | 20      | 0            |
| 21  | Aa    | 867   | 0        | 920      | 30      | 0            |
| 22  | Ab    | 653   | 0        | 680      | 24      | 0            |
| 23  | AD    | 1782  | 0        | 1862     | 46      | 0            |
| 24  | Ae    | 469   | 0        | 503      | 19      | 0            |
| 25  | Af    | 659   | 0        | 695      | 19      | 0            |
| 26  | AJ    | 1503  | 0        | 1620     | 56      | 0            |
| 27  | Ca    | 1204  | 0        | 1260     | 59      | 0            |
| 28  | CN    | 1710  | 0        | 1778     | 106     | 0            |
| 29  | CI    | 1785  | 0        | 1805     | 59      | 0            |
| 30  | CD    | 2334  | 0        | 2354     | 75      | 0            |
| 31  | CQ    | 1518  | 0        | 1626     | 54      | 0            |
| 32  | CR    | 1683  | 0        | 1827     | 43      | 0            |
| 33  | CS    | 1454  | 0        | 1503     | 66      | 0            |
| 34  | CT    | 1297  | 0        | 1364     | 54      | 0            |
| 35  | CP    | 1505  | 0        | 1556     | 50      | 0            |
| 36  | CX    | 984   | 0        | 1058     | 37      | 0            |
| 37  | CY    | 1078  | 0        | 1159     | 34      | 0            |
| 38  | CZ    | 1115  | 0        | 1199     | 44      | 0            |
| 39  | Cr    | 1051  | 0        | 1148     | 42      | 0            |
| 40  | Ch    | 1015  | 0        | 1163     | 36      | 0            |
| 41  | Cb    | 619   | 0        | 650      | 15      | 0            |
| 42  | Cc    | 770   | 0        | 802      | 23      | 0            |
| 43  | Cd    | 924   | 0        | 942      | 23      | 0            |
| 44  | Ce    | 1110  | 0        | 1181     | 33      | 0            |
| 45  | Cf    | 1244  | 0        | 1316     | 60      | 0            |
| 46  | Ci    | 934   | 0        | 1029     | 44      | 0            |
| 47  | Ck    | 576   | 0        | 634      | 23      | 0            |
| 48  | Cl    | 437   | 0        | 483      | 24      | 0            |
| 49  | Cm    | 429   | 0        | 472      | 11      | 0            |
| 50  | Cn    | 236   | 0        | 286      | 6       | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 51  | Cp    | 710    | 0        | 756      | 23      | 0            |
| 52  | Co    | 874    | 0        | 956      | 20      | 0            |
| 53  | CJ    | 1468   | 0        | 1507     | 47      | 0            |
| 54  | CH    | 1499   | 0        | 1569     | 52      | 0            |
| 55  | CE    | 1845   | 0        | 1981     | 79      | 0            |
| 56  | CG    | 1936   | 0        | 2103     | 50      | 0            |
| 57  | A9    | 639    | 0        | 321      | 13      | 0            |
| 58  | A7    | 2554   | 0        | 1296     | 52      | 0            |
| 59  | A8    | 2621   | 0        | 1327     | 79      | 0            |
| 60  | Cz    | 1702   | 0        | 1814     | 37      | 0            |
| 61  | B2    | 39355  | 0        | 19531    | 807     | 0            |
| 62  | A5    | 77175  | 0        | 38515    | 1442    | 0            |
| 63  | Ac    | 498    | 0        | 525      | 19      | 0            |
| 64  | AW    | 1028   | 0        | 1071     | 47      | 0            |
| 65  | CW    | 483    | 0        | 510      | 9       | 0            |
| 66  | Cg    | 852    | 0        | 933      | 39      | 0            |
| 67  | CU    | 811    | 0        | 838      | 22      | 0            |
| 68  | AK    | 760    | 0        | 757      | 20      | 0            |
| 69  | AT    | 1041   | 0        | 1061     | 409     | 0            |
| 70  | AF    | 1490   | 0        | 1548     | 60      | 0            |
| 71  | CF    | 1895   | 0        | 2012     | 54      | 0            |
| 72  | AE    | 2054   | 0        | 2165     | 70      | 0            |
| 73  | AG    | 1866   | 0        | 2029     | 62      | 0            |
| 74  | AH    | 1566   | 0        | 1664     | 59      | 0            |
| 75  | AI    | 1665   | 0        | 1746     | 61      | 0            |
| 76  | AQ    | 1183   | 0        | 1255     | 46      | 0            |
| 77  | CO    | 1668   | 0        | 1783     | 70      | 0            |
| 78  | CL    | 1695   | 0        | 1790     | 71      | 0            |
| 79  | CV    | 998    | 0        | 1046     | 32      | 0            |
| 80  | CM    | 1302   | 0        | 1388     | 65      | 0            |
| 81  | B     | 1605   | 0        | 814      | 22      | 0            |
| 82  | v     | 255    | 0        | 130      | 2       | 0            |
| 83  | Cj    | 696    | 0        | 720      | 102     | 0            |
| All | All   | 219005 | 0        | 161752   | 5054    | 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 15.

All (5054) 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) |
|-------------------|-------------------|--------------------------|-------------------|
| 61:B2:1717:A:H4'  | 69:AT:92:PHE:CE1  | 1.20                     | 1.70              |
| 62:A5:1017:A:C8   | 83:Cj:15:THR:HG22 | 1.21                     | 1.70              |
| 59:A8:107:U:C5    | 83:Cj:20:ARG:HD2  | 1.25                     | 1.69              |
| 69:AT:29:LYS:CD   | 69:AT:106:ALA:HA  | 1.24                     | 1.67              |
| 62:A5:1017:A:H8   | 83:Cj:15:THR:CG2  | 1.15                     | 1.59              |
| 69:AT:29:LYS:HD2  | 69:AT:106:ALA:CA  | 1.30                     | 1.56              |
| 12:AS:39:ARG:CG   | 69:AT:38:LYS:NZ   | 1.71                     | 1.53              |
| 61:B2:1727:U:C5   | 61:B2:1727:U:C6   | 1.99                     | 1.50              |
| 12:AS:39:ARG:HG2  | 69:AT:38:LYS:NZ   | 1.12                     | 1.44              |
| 59:A8:107:U:H5    | 83:Cj:20:ARG:CD   | 1.32                     | 1.42              |
| 69:AT:72:VAL:CG1  | 69:AT:101:ARG:HE  | 1.31                     | 1.41              |
| 69:AT:72:VAL:HG11 | 69:AT:101:ARG:NE  | 1.28                     | 1.41              |
| 69:AT:75:ILE:O    | 69:AT:79:TYR:CD2  | 1.72                     | 1.40              |
| 69:AT:136:ASN:O   | 69:AT:140:PHE:CD2 | 1.76                     | 1.39              |
| 12:AS:83:PHE:CE2  | 69:AT:36:ILE:HG21 | 1.58                     | 1.38              |
| 61:B2:1717:A:C4'  | 69:AT:92:PHE:HE1  | 1.36                     | 1.38              |
| 61:B2:1715:G:C6   | 69:AT:67:ARG:HG3  | 1.59                     | 1.37              |
| 69:AT:61:LEU:CD2  | 69:AT:132:ASP:OD2 | 1.72                     | 1.36              |
| 69:AT:72:VAL:HG11 | 69:AT:101:ARG:CD  | 1.57                     | 1.33              |
| 61:B2:1727:U:C5   | 61:B2:1727:U:C4   | 2.16                     | 1.32              |
| 69:AT:75:ILE:C    | 69:AT:79:TYR:HD2  | 1.37                     | 1.32              |
| 61:B2:1717:A:C4'  | 69:AT:92:PHE:CE1  | 2.09                     | 1.31              |
| 62:A5:1017:A:C8   | 83:Cj:15:THR:CG2  | 1.95                     | 1.30              |
| 69:AT:72:VAL:CG1  | 69:AT:101:ARG:NE  | 1.92                     | 1.29              |
| 59:A8:107:U:C5    | 83:Cj:20:ARG:CD   | 2.11                     | 1.29              |
| 69:AT:75:ILE:O    | 69:AT:79:TYR:HD2  | 0.96                     | 1.28              |
| 61:B2:1716:A:OP1  | 69:AT:78:ILE:CG2  | 1.81                     | 1.27              |
| 61:B2:1782:G:O3'  | 69:AT:92:PHE:HE2  | 1.16                     | 1.26              |
| 69:AT:75:ILE:HG23 | 69:AT:79:TYR:CE2  | 1.71                     | 1.25              |
| 61:B2:1445:A:O4'  | 69:AT:129:ARG:CZ  | 1.68                     | 1.24              |
| 61:B2:1715:G:C5'  | 69:AT:78:ILE:HD13 | 1.67                     | 1.23              |
| 61:B2:1715:G:C6   | 69:AT:67:ARG:CG   | 2.21                     | 1.21              |
| 69:AT:72:VAL:HG11 | 69:AT:101:ARG:CG  | 1.68                     | 1.21              |
| 59:A8:34:C:OP1    | 83:Cj:70:LEU:HD11 | 1.11                     | 1.21              |
| 61:B2:1715:G:O5'  | 69:AT:78:ILE:CD1  | 1.87                     | 1.20              |
| 69:AT:61:LEU:CA   | 69:AT:65:TYR:HE2  | 1.52                     | 1.19              |
| 69:AT:136:ASN:O   | 69:AT:140:PHE:HD2 | 1.11                     | 1.19              |
| 59:A8:34:C:OP1    | 83:Cj:70:LEU:CD1  | 1.91                     | 1.19              |
| 69:AT:75:ILE:HA   | 69:AT:79:TYR:CE2  | 1.77                     | 1.19              |
| 69:AT:75:ILE:C    | 69:AT:79:TYR:CD2  | 2.16                     | 1.18              |
| 62:A5:2518:A:C8   | 83:Cj:3:LYS:HE2   | 1.79                     | 1.18              |
| 12:AS:83:PHE:CE2  | 69:AT:36:ILE:CG2  | 2.27                     | 1.18              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 69:AT:61:LEU:HD21  | 69:AT:132:ASP:CG   | 1.70                     | 1.17              |
| 69:AT:61:LEU:HA    | 69:AT:65:TYR:CE2   | 1.74                     | 1.16              |
| 69:AT:143:ARG:O    | 69:AT:147:LYS:HG3  | 1.42                     | 1.16              |
| 61:B2:1693:C:OP1   | 69:AT:102:LYS:CE   | 1.94                     | 1.16              |
| 61:B2:1727:U:C6    | 61:B2:1727:U:N1    | 2.14                     | 1.15              |
| 61:B2:1782:G:O3'   | 69:AT:92:PHE:CE2   | 1.99                     | 1.14              |
| 61:B2:1445:A:H4'   | 69:AT:129:ARG:HD3  | 1.20                     | 1.14              |
| 69:AT:42:PHE:CE1   | 69:AT:85:ASN:OD1   | 2.01                     | 1.13              |
| 61:B2:1667:A:H5''  | 69:AT:84:ARG:NH1   | 1.64                     | 1.13              |
| 59:A8:67:G:H5'     | 83:Cj:87:LYS:HG3   | 1.31                     | 1.12              |
| 61:B2:1717:A:H4'   | 69:AT:92:PHE:CZ    | 1.85                     | 1.11              |
| 61:B2:1727:U:N3    | 61:B2:1727:U:C2    | 2.18                     | 1.10              |
| 61:B2:1695:A:H5''  | 69:AT:33:GLN:HE22  | 1.13                     | 1.10              |
| 61:B2:1727:U:N1    | 61:B2:1727:U:C2    | 2.20                     | 1.10              |
| 61:B2:1727:U:C4    | 61:B2:1727:U:N3    | 2.20                     | 1.09              |
| 69:AT:126:ILE:CG2  | 69:AT:131:LEU:HG   | 1.80                     | 1.09              |
| 69:AT:126:ILE:HG22 | 69:AT:131:LEU:CG   | 1.83                     | 1.09              |
| 62:A5:2518:A:N7    | 83:Cj:3:LYS:HE3    | 1.67                     | 1.09              |
| 12:AS:39:ARG:HG3   | 69:AT:38:LYS:NZ    | 1.63                     | 1.09              |
| 69:AT:38:LYS:O     | 69:AT:43:LYS:HD2   | 1.53                     | 1.09              |
| 62:A5:2518:A:N7    | 83:Cj:3:LYS:CE     | 2.16                     | 1.08              |
| 61:B2:1715:G:C5'   | 69:AT:78:ILE:CD1   | 2.30                     | 1.08              |
| 61:B2:1696:G:O3'   | 69:AT:41:LYS:HE3   | 1.23                     | 1.08              |
| 69:AT:17:ALA:O     | 69:AT:21:PHE:CD2   | 2.06                     | 1.08              |
| 69:AT:61:LEU:HD21  | 69:AT:132:ASP:OD2  | 1.50                     | 1.08              |
| 61:B2:1670:G:O6    | 69:AT:82:ARG:NH1   | 1.87                     | 1.07              |
| 69:AT:61:LEU:HA    | 69:AT:65:TYR:HE2   | 0.92                     | 1.07              |
| 61:B2:1670:G:O2'   | 69:AT:52:TRP:CE3   | 2.06                     | 1.07              |
| 69:AT:15:THR:HB    | 69:AT:55:VAL:CG1   | 1.85                     | 1.07              |
| 69:AT:72:VAL:HG12  | 69:AT:101:ARG:HE   | 1.19                     | 1.07              |
| 61:B2:1715:G:H5'   | 69:AT:78:ILE:HD13  | 1.37                     | 1.07              |
| 69:AT:75:ILE:CA    | 69:AT:79:TYR:CE2   | 2.37                     | 1.06              |
| 12:AS:83:PHE:CZ    | 69:AT:36:ILE:CG2   | 2.38                     | 1.05              |
| 69:AT:75:ILE:HA    | 69:AT:79:TYR:HE2   | 0.94                     | 1.05              |
| 61:B2:1671:U:H3    | 69:AT:82:ARG:NH2   | 1.52                     | 1.05              |
| 62:A5:2168:G:C2    | 83:Cj:9:GLY:HA3    | 1.92                     | 1.05              |
| 69:AT:60:ILE:CG2   | 69:AT:64:LEU:HG    | 1.85                     | 1.05              |
| 62:A5:1017:A:H8    | 83:Cj:15:THR:HG21  | 1.19                     | 1.04              |
| 69:AT:50:PRO:HA    | 69:AT:53:PHE:CE2   | 1.93                     | 1.04              |
| 69:AT:42:PHE:CD1   | 69:AT:85:ASN:OD1   | 2.10                     | 1.04              |
| 69:AT:70:ALA:O     | 69:AT:123:LEU:HD11 | 1.57                     | 1.04              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 69:AT:75:ILE:CA   | 69:AT:79:TYR:HE2  | 1.70                     | 1.04              |
| 61:B2:1693:C:OP1  | 69:AT:102:LYS:HE2 | 1.55                     | 1.03              |
| 61:B2:1695:A:H4'  | 69:AT:33:GLN:OE1  | 1.58                     | 1.03              |
| 69:AT:6:VAL:HG21  | 69:AT:136:ASN:OD1 | 1.58                     | 1.03              |
| 69:AT:75:ILE:CG2  | 69:AT:79:TYR:CE2  | 2.41                     | 1.03              |
| 69:AT:60:ILE:HG23 | 69:AT:64:LEU:HG   | 1.05                     | 1.03              |
| 59:A8:67:G:H5'    | 83:Cj:87:LYS:CG   | 1.82                     | 1.03              |
| 42:Cc:51:ASN:H    | 42:Cc:51:ASN:HD22 | 1.03                     | 1.03              |
| 61:B2:1755:A:H4'  | 69:AT:41:LYS:HD3  | 1.38                     | 1.03              |
| 62:A5:2160:C:H1'  | 83:Cj:8:PHE:O     | 1.59                     | 1.01              |
| 61:B2:1540:G:O5'  | 69:AT:7:LYS:NZ    | 1.92                     | 1.01              |
| 61:B2:1667:A:H5'' | 69:AT:84:ARG:HH12 | 1.17                     | 1.01              |
| 69:AT:61:LEU:CD2  | 69:AT:132:ASP:CG  | 2.29                     | 1.00              |
| 69:AT:61:LEU:HD22 | 69:AT:132:ASP:OD2 | 1.60                     | 0.99              |
| 62:A5:1017:A:N7   | 83:Cj:15:THR:HG22 | 1.77                     | 0.99              |
| 61:B2:1716:A:OP1  | 69:AT:78:ILE:HG23 | 1.59                     | 0.99              |
| 69:AT:72:VAL:CG1  | 69:AT:101:ARG:HG2 | 1.93                     | 0.98              |
| 61:B2:1445:A:H4'  | 69:AT:129:ARG:CD  | 1.92                     | 0.98              |
| 59:A8:56:U:H5     | 83:Cj:63:ARG:NH2  | 1.61                     | 0.98              |
| 69:AT:49:ASP:HB3  | 69:AT:50:PRO:HD3  | 1.44                     | 0.98              |
| 61:B2:1445:A:O2'  | 69:AT:133:ARG:CZ  | 2.12                     | 0.97              |
| 69:AT:42:PHE:CE1  | 69:AT:85:ASN:CG   | 2.42                     | 0.97              |
| 69:AT:60:ILE:HG23 | 69:AT:64:LEU:CG   | 1.94                     | 0.97              |
| 62:A5:2518:A:C8   | 83:Cj:3:LYS:CE    | 2.47                     | 0.97              |
| 59:A8:56:U:C5     | 83:Cj:63:ARG:NH2  | 2.33                     | 0.96              |
| 62:A5:56:A:H5'    | 83:Cj:48:ASN:HB2  | 1.46                     | 0.96              |
| 61:B2:1715:G:C2   | 69:AT:67:ARG:HG2  | 2.01                     | 0.96              |
| 61:B2:1716:A:OP1  | 69:AT:78:ILE:HG22 | 1.66                     | 0.96              |
| 61:B2:1540:G:C5'  | 69:AT:7:LYS:HZ2   | 1.78                     | 0.96              |
| 61:B2:1695:A:H5'' | 69:AT:33:GLN:NE2  | 1.79                     | 0.95              |
| 61:B2:1540:G:H22  | 69:AT:129:ARG:NH2 | 1.64                     | 0.95              |
| 69:AT:17:ALA:O    | 69:AT:21:PHE:CE2  | 2.20                     | 0.95              |
| 61:B2:1715:G:H5'  | 69:AT:78:ILE:CD1  | 1.93                     | 0.95              |
| 61:B2:1445:A:C4'  | 69:AT:129:ARG:HD3 | 1.97                     | 0.95              |
| 69:AT:72:VAL:CG1  | 69:AT:101:ARG:CG  | 2.44                     | 0.94              |
| 61:B2:1671:U:O4   | 69:AT:82:ARG:CZ   | 2.15                     | 0.94              |
| 12:AS:39:ARG:CG   | 69:AT:38:LYS:HZ2  | 1.51                     | 0.94              |
| 69:AT:59:SER:HB2  | 69:AT:63:HIS:CD2  | 2.03                     | 0.94              |
| 69:AT:54:TYR:HE1  | 69:AT:103:ALA:CB  | 1.81                     | 0.94              |
| 69:AT:29:LYS:CE   | 69:AT:106:ALA:HA  | 1.98                     | 0.93              |
| 12:AS:83:PHE:HE2  | 69:AT:36:ILE:HG21 | 1.20                     | 0.93              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 62:A5:1016:A:OP1   | 83:Cj:28:HIS:NE2  | 2.01                     | 0.92              |
| 61:B2:1715:G:C5    | 69:AT:67:ARG:CG   | 2.52                     | 0.92              |
| 61:B2:1667:A:C5'   | 69:AT:84:ARG:HH12 | 1.83                     | 0.91              |
| 69:AT:126:ILE:HG22 | 69:AT:131:LEU:HG  | 0.92                     | 0.91              |
| 69:AT:72:VAL:CG2   | 69:AT:101:ARG:HG2 | 2.01                     | 0.91              |
| 61:B2:1696:G:O3'   | 69:AT:41:LYS:CE   | 2.17                     | 0.91              |
| 69:AT:76:THR:HB    | 69:AT:97:ASP:OD1  | 1.72                     | 0.90              |
| 69:AT:76:THR:CB    | 69:AT:97:ASP:OD1  | 2.03                     | 0.90              |
| 61:B2:1445:A:OP1   | 69:AT:129:ARG:HD2 | 1.71                     | 0.90              |
| 69:AT:23:LYS:HG2   | 69:AT:28:LEU:CD2  | 2.01                     | 0.90              |
| 61:B2:1445:A:P     | 69:AT:129:ARG:HD2 | 2.12                     | 0.90              |
| 69:AT:61:LEU:CA    | 69:AT:65:TYR:CE2  | 2.30                     | 0.90              |
| 61:B2:1670:G:OP1   | 69:AT:43:LYS:NZ   | 2.04                     | 0.89              |
| 61:B2:1715:G:N1    | 69:AT:67:ARG:CG   | 2.36                     | 0.89              |
| 61:B2:1727:U:C6    | 70:AF:190:ILE:HB  | 2.06                     | 0.89              |
| 61:B2:1727:U:N1    | 70:AF:190:ILE:HB  | 1.86                     | 0.89              |
| 69:AT:17:ALA:C     | 69:AT:21:PHE:CE2  | 2.51                     | 0.88              |
| 42:Cc:51:ASN:H     | 42:Cc:51:ASN:ND2  | 1.61                     | 0.88              |
| 69:AT:18:VAL:HA    | 69:AT:21:PHE:HD2  | 1.38                     | 0.88              |
| 48:Cl:8:ARG:NH2    | 83:Cj:20:ARG:NE   | 2.20                     | 0.88              |
| 59:A8:67:G:C5'     | 83:Cj:87:LYS:HG3  | 1.97                     | 0.88              |
| 61:B2:1715:G:O5'   | 69:AT:78:ILE:HD13 | 1.62                     | 0.88              |
| 61:B2:1716:A:P     | 69:AT:78:ILE:HG23 | 2.13                     | 0.88              |
| 69:AT:61:LEU:HD21  | 69:AT:132:ASP:OD1 | 1.75                     | 0.87              |
| 42:Cc:51:ASN:HD22  | 42:Cc:51:ASN:N    | 1.67                     | 0.87              |
| 69:AT:54:TYR:HE1   | 69:AT:103:ALA:HB2 | 1.39                     | 0.87              |
| 69:AT:75:ILE:CG2   | 69:AT:79:TYR:CD2  | 2.57                     | 0.87              |
| 61:B2:1445:A:O2'   | 69:AT:133:ARG:NH1 | 2.08                     | 0.87              |
| 58:A7:75:G:HO2'    | 58:A7:99:G:H1     | 1.20                     | 0.87              |
| 61:B2:1660:U:O4'   | 69:AT:88:HIS:CE1  | 2.28                     | 0.86              |
| 62:A5:1121:A:C2    | 83:Cj:8:PHE:CZ    | 2.62                     | 0.86              |
| 69:AT:15:THR:HB    | 69:AT:55:VAL:HG13 | 1.55                     | 0.86              |
| 69:AT:15:THR:HB    | 69:AT:55:VAL:HG11 | 1.54                     | 0.86              |
| 61:B2:1445:A:C4'   | 69:AT:133:ARG:NH2 | 2.39                     | 0.86              |
| 69:AT:49:ASP:HB3   | 69:AT:50:PRO:CD   | 2.05                     | 0.86              |
| 61:B2:1717:A:C5'   | 69:AT:92:PHE:HE1  | 1.88                     | 0.85              |
| 69:AT:11:GLN:HB3   | 69:AT:15:THR:HG23 | 1.58                     | 0.85              |
| 69:AT:144:ASP:HA   | 69:AT:147:LYS:CD  | 2.06                     | 0.85              |
| 61:B2:1445:A:O4'   | 69:AT:129:ARG:NE  | 2.10                     | 0.84              |
| 69:AT:50:PRO:HA    | 69:AT:53:PHE:HE2  | 1.39                     | 0.84              |
| 61:B2:1445:A:C4'   | 69:AT:129:ARG:CD  | 2.54                     | 0.84              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:CA:4:VAL:HG13   | 2:CA:8:GLN:HB2     | 1.60                     | 0.84              |
| 61:B2:1540:G:H22  | 69:AT:129:ARG:HH21 | 1.25                     | 0.84              |
| 69:AT:50:PRO:HA   | 69:AT:53:PHE:CD2   | 2.12                     | 0.84              |
| 69:AT:29:LYS:CD   | 69:AT:106:ALA:CA   | 2.14                     | 0.83              |
| 69:AT:64:LEU:CD2  | 69:AT:69:PRO:HA    | 2.09                     | 0.83              |
| 62:A5:2518:A:H8   | 83:Cj:3:LYS:HE2    | 1.39                     | 0.83              |
| 69:AT:50:PRO:O    | 69:AT:53:PHE:HD2   | 1.61                     | 0.83              |
| 61:B2:1540:G:N2   | 69:AT:129:ARG:HH21 | 1.77                     | 0.82              |
| 61:B2:1716:A:P    | 69:AT:78:ILE:CG2   | 2.67                     | 0.82              |
| 69:AT:75:ILE:HG23 | 69:AT:79:TYR:CZ    | 2.14                     | 0.81              |
| 61:B2:1671:U:N3   | 69:AT:82:ARG:NH2   | 2.28                     | 0.81              |
| 61:B2:1715:G:N1   | 69:AT:67:ARG:HG3   | 1.93                     | 0.81              |
| 61:B2:1540:G:C5'  | 69:AT:7:LYS:NZ     | 2.44                     | 0.81              |
| 61:B2:1540:G:H22  | 69:AT:129:ARG:CZ   | 1.92                     | 0.81              |
| 62:A5:2160:C:O2   | 83:Cj:8:PHE:O      | 1.97                     | 0.81              |
| 62:A5:1085:U:OP1  | 83:Cj:6:THR:HG21   | 1.81                     | 0.81              |
| 69:AT:136:ASN:HB3 | 69:AT:140:PHE:HE2  | 1.45                     | 0.81              |
| 69:AT:60:ILE:CG2  | 69:AT:64:LEU:CG    | 2.55                     | 0.81              |
| 61:B2:1445:A:H4'  | 69:AT:133:ARG:NH2  | 1.96                     | 0.80              |
| 61:B2:1717:A:C4'  | 69:AT:92:PHE:CZ    | 2.56                     | 0.80              |
| 69:AT:29:LYS:HD2  | 69:AT:106:ALA:CB   | 2.10                     | 0.80              |
| 61:B2:1715:G:O5'  | 69:AT:78:ILE:HD11  | 1.79                     | 0.80              |
| 69:AT:72:VAL:HG21 | 69:AT:101:ARG:HG2  | 1.63                     | 0.80              |
| 69:AT:60:ILE:CG2  | 69:AT:64:LEU:CD1   | 2.59                     | 0.80              |
| 62:A5:3609:A:N6   | 62:A5:3615:G:N7    | 2.30                     | 0.79              |
| 69:AT:75:ILE:HG23 | 69:AT:79:TYR:CD2   | 2.16                     | 0.79              |
| 69:AT:54:TYR:CE1  | 69:AT:103:ALA:CB   | 2.65                     | 0.79              |
| 69:AT:136:ASN:C   | 69:AT:140:PHE:HD2  | 1.91                     | 0.79              |
| 61:B2:1320:G:H1   | 61:B2:1339:C:H42   | 1.28                     | 0.79              |
| 62:A5:117:C:H42   | 62:A5:285:G:H1     | 1.29                     | 0.79              |
| 61:B2:1715:G:C6   | 69:AT:67:ARG:HG2   | 2.18                     | 0.79              |
| 62:A5:1311:U:H2'  | 62:A5:1312:G:H8    | 1.46                     | 0.79              |
| 69:AT:144:ASP:HA  | 69:AT:147:LYS:HD2  | 1.64                     | 0.79              |
| 69:AT:6:VAL:HG11  | 69:AT:136:ASN:OD1  | 1.82                     | 0.78              |
| 61:B2:108:G:H1    | 61:B2:310:C:H42    | 1.31                     | 0.78              |
| 61:B2:1445:A:H4'  | 69:AT:133:ARG:HH12 | 1.47                     | 0.78              |
| 6:CC:48:ARG:NH2   | 62:A5:356:A:N7     | 2.32                     | 0.78              |
| 61:B2:1715:G:N1   | 69:AT:67:ARG:HG2   | 1.96                     | 0.77              |
| 69:AT:72:VAL:CG1  | 69:AT:101:ARG:CD   | 2.50                     | 0.77              |
| 62:A5:56:A:C5'    | 83:Cj:48:ASN:HB2   | 2.14                     | 0.77              |
| 69:AT:39:THR:O    | 69:AT:40:ALA:CB    | 2.33                     | 0.77              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 61:B2:1445:A:O4'  | 69:AT:133:ARG:NH2 | 2.18                     | 0.77              |
| 62:A5:1538:U:H2'  | 62:A5:1539:A:H8   | 1.51                     | 0.76              |
| 69:AT:39:THR:OG1  | 69:AT:43:LYS:NZ   | 2.14                     | 0.76              |
| 62:A5:3591:A:O2'  | 62:A5:3620:G:N2   | 2.19                     | 0.76              |
| 69:AT:11:GLN:OE1  | 69:AT:58:ALA:HB1  | 1.86                     | 0.76              |
| 59:A8:12:G:H1     | 62:A5:428:C:H42   | 1.30                     | 0.76              |
| 61:B2:1740:G:N2   | 61:B2:1756:C:N3   | 2.33                     | 0.76              |
| 69:AT:17:ALA:C    | 69:AT:21:PHE:HE2  | 1.93                     | 0.75              |
| 2:CA:207:VAL:HG23 | 2:CA:208:GLU:HG3  | 1.69                     | 0.75              |
| 62:A5:1383:A:N6   | 62:A5:1545:A:N7   | 2.35                     | 0.75              |
| 69:AT:23:LYS:HA   | 69:AT:28:LEU:CD2  | 2.16                     | 0.75              |
| 61:B2:636:G:H21   | 61:B2:1058:A:H62  | 1.31                     | 0.75              |
| 69:AT:17:ALA:HB1  | 69:AT:21:PHE:HE2  | 1.49                     | 0.75              |
| 59:A8:36:A:N6     | 62:A5:25:G:N7     | 2.35                     | 0.75              |
| 62:A5:2160:C:O2   | 83:Cj:8:PHE:C     | 2.30                     | 0.75              |
| 61:B2:1972:G:H1   | 61:B2:1979:C:H42  | 1.35                     | 0.74              |
| 69:AT:18:VAL:HA   | 69:AT:21:PHE:CD2  | 2.22                     | 0.74              |
| 12:AS:83:PHE:CZ   | 69:AT:36:ILE:HG23 | 2.21                     | 0.74              |
| 59:A8:92:G:OP2    | 83:Cj:72:ARG:HD2  | 1.87                     | 0.74              |
| 62:A5:56:A:H5'    | 83:Cj:48:ASN:CB   | 2.16                     | 0.74              |
| 61:B2:1444:C:H2'  | 69:AT:129:ARG:NE  | 2.02                     | 0.74              |
| 61:B2:1727:U:C2   | 70:AF:190:ILE:CG1 | 2.71                     | 0.74              |
| 61:B2:1782:G:C3'  | 69:AT:92:PHE:HE2  | 2.00                     | 0.74              |
| 61:B2:1755:A:H4'  | 69:AT:41:LYS:CD   | 2.17                     | 0.74              |
| 62:A5:44:A:H61    | 62:A5:1163:G:H21  | 1.35                     | 0.74              |
| 62:A5:362:A:H61   | 62:A5:367:A:H62   | 1.33                     | 0.74              |
| 55:CE:237:TYR:HB2 | 55:CE:241:MET:HB2 | 1.70                     | 0.73              |
| 62:A5:78:A:H5''   | 78:CL:104:LYS:HE2 | 1.70                     | 0.73              |
| 69:AT:63:HIS:CE1  | 69:AT:67:ARG:CZ   | 2.71                     | 0.73              |
| 69:AT:37:VAL:HG12 | 69:AT:39:THR:H    | 1.53                     | 0.73              |
| 9:AO:146:ARG:HD3  | 21:Aa:29:CYS:HB3  | 1.70                     | 0.73              |
| 69:AT:54:TYR:CE1  | 69:AT:103:ALA:HB2 | 2.22                     | 0.73              |
| 61:B2:1715:G:C4   | 69:AT:67:ARG:HG2  | 2.24                     | 0.72              |
| 62:A5:33:C:N3     | 62:A5:34:C:N4     | 2.38                     | 0.72              |
| 46:Ci:43:GLN:HE22 | 46:Ci:48:LYS:HB2  | 1.52                     | 0.72              |
| 69:AT:39:THR:O    | 69:AT:40:ALA:HB2  | 1.88                     | 0.72              |
| 69:AT:143:ARG:O   | 69:AT:147:LYS:CG  | 2.32                     | 0.72              |
| 62:A5:1549:A:H5'' | 71:CF:216:LYS:HB3 | 1.69                     | 0.72              |
| 61:B2:1444:C:H2'  | 69:AT:129:ARG:HE  | 1.54                     | 0.71              |
| 61:B2:1302:U:H3   | 61:B2:1641:U:H3   | 1.35                     | 0.71              |
| 62:A5:1153:G:N2   | 62:A5:1329:G:OP1  | 2.23                     | 0.71              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 5:AC:106:ARG:HD3  | 5:AC:126:CYS:HB3   | 1.72                     | 0.71              |
| 62:A5:709:U:H3    | 62:A5:727:G:H1     | 1.38                     | 0.71              |
| 62:A5:788:C:N4    | 62:A5:797:A:OP1    | 2.24                     | 0.71              |
| 69:AT:64:LEU:HD22 | 69:AT:69:PRO:HA    | 1.72                     | 0.71              |
| 1:AA:102:ARG:HE   | 1:AA:104:THR:H     | 1.38                     | 0.70              |
| 69:AT:17:ALA:HB1  | 69:AT:21:PHE:CE2   | 2.26                     | 0.70              |
| 69:AT:75:ILE:CA   | 69:AT:79:TYR:CD2   | 2.68                     | 0.70              |
| 37:CY:15:ARG:NH2  | 59:A8:22:C:OP1     | 2.24                     | 0.70              |
| 61:B2:1755:A:C4'  | 69:AT:41:LYS:HD3   | 2.19                     | 0.70              |
| 65:CW:6:CYS:SG    | 65:CW:7:ALA:N      | 2.65                     | 0.70              |
| 59:A8:67:G:C5'    | 83:Cj:87:LYS:CG    | 2.27                     | 0.70              |
| 59:A8:67:G:O2'    | 83:Cj:87:LYS:NZ    | 2.25                     | 0.70              |
| 35:CP:127:ARG:NH2 | 62:A5:2733:G:OP1   | 2.24                     | 0.70              |
| 62:A5:2624:G:H2'  | 62:A5:2625:G:H8    | 1.55                     | 0.70              |
| 33:CS:164:ARG:HD2 | 45:Cf:43:LYS:HD2   | 1.72                     | 0.70              |
| 61:B2:78:A:H61    | 73:AG:154:ARG:HH22 | 1.36                     | 0.70              |
| 69:AT:59:SER:C    | 69:AT:63:HIS:HD2   | 2.00                     | 0.70              |
| 69:AT:75:ILE:CB   | 69:AT:79:TYR:CE2   | 2.75                     | 0.70              |
| 69:AT:72:VAL:HG21 | 69:AT:101:ARG:CG   | 2.21                     | 0.70              |
| 76:AQ:78:GLY:H    | 76:AQ:82:GLN:HB2   | 1.57                     | 0.70              |
| 37:CY:8:SER:OG    | 37:CY:9:SER:N      | 2.23                     | 0.70              |
| 6:CC:103:ARG:NH2  | 62:A5:1004:C:OP1   | 2.24                     | 0.69              |
| 62:A5:2168:G:N3   | 83:Cj:9:GLY:HA3    | 2.05                     | 0.69              |
| 69:AT:6:VAL:CG2   | 69:AT:136:ASN:OD1  | 2.37                     | 0.69              |
| 61:B2:1445:A:H4'  | 69:AT:133:ARG:NH1  | 2.06                     | 0.69              |
| 25:Af:78:LYS:HB3  | 61:B2:1638:A:H4'   | 1.73                     | 0.69              |
| 62:A5:1383:A:N7   | 62:A5:1545:A:N6    | 2.39                     | 0.69              |
| 62:A5:1388:C:O2   | 62:A5:1526:G:N2    | 2.23                     | 0.69              |
| 62:A5:2161:G:O2'  | 83:Cj:5:THR:HG23   | 1.91                     | 0.69              |
| 69:AT:129:ARG:HB3 | 69:AT:133:ARG:CZ   | 2.22                     | 0.69              |
| 61:B2:1660:U:C1'  | 69:AT:88:HIS:HE1   | 2.05                     | 0.69              |
| 33:CS:173:ARG:NH2 | 62:A5:3726:U:O4    | 2.26                     | 0.69              |
| 47:Ck:10:ASP:HA   | 47:Ck:13:ASN:HB3   | 1.74                     | 0.69              |
| 56:CG:58:ARG:NH1  | 62:A5:3117:A:N7    | 2.40                     | 0.69              |
| 62:A5:2774:G:O6   | 62:A5:3515:C:N4    | 2.25                     | 0.69              |
| 33:CS:176:PHE:HB2 | 62:A5:3753:A:H4'   | 1.74                     | 0.69              |
| 62:A5:1689:G:N2   | 62:A5:2734:A:OP2   | 2.25                     | 0.69              |
| 62:A5:2129:C:H4'  | 62:A5:2130:G:H4'   | 1.74                     | 0.69              |
| 69:AT:59:SER:O    | 69:AT:63:HIS:CD2   | 2.45                     | 0.69              |
| 59:A8:4:U:O2      | 62:A5:437:G:N2     | 2.25                     | 0.69              |
| 69:AT:23:LYS:HA   | 69:AT:28:LEU:HD23  | 1.75                     | 0.69              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 61:B2:1689:A:OP1   | 69:AT:77:LYS:NZ    | 2.26                     | 0.69              |
| 62:A5:3716:C:N3    | 62:A5:3762:G:N1    | 2.41                     | 0.69              |
| 55:CE:223:ALA:H    | 55:CE:225:TYR:HD2  | 1.40                     | 0.68              |
| 34:CT:61:THR:HG21  | 62:A5:1272:G:H21   | 1.58                     | 0.68              |
| 69:AT:6:VAL:HG21   | 69:AT:136:ASN:CG   | 2.18                     | 0.68              |
| 69:AT:23:LYS:CB    | 69:AT:28:LEU:HD21  | 2.23                     | 0.68              |
| 69:AT:50:PRO:HD2   | 69:AT:51:ASP:N     | 2.07                     | 0.68              |
| 45:Cf:134:ARG:HH12 | 62:A5:1379:U:H5'   | 1.57                     | 0.68              |
| 62:A5:1015:G:N2    | 62:A5:1120:A:OP2   | 2.24                     | 0.68              |
| 69:AT:59:SER:C     | 69:AT:63:HIS:CD2   | 2.71                     | 0.68              |
| 69:AT:64:LEU:HD21  | 69:AT:123:LEU:HD12 | 1.76                     | 0.68              |
| 30:CD:21:ARG:NH1   | 58:A7:110:G:N7     | 2.42                     | 0.68              |
| 61:B2:1695:A:C4'   | 69:AT:33:GLN:OE1   | 2.37                     | 0.68              |
| 62:A5:1334:A:N6    | 62:A5:1352:U:O4    | 2.26                     | 0.68              |
| 61:B2:1540:G:H22   | 69:AT:129:ARG:NE   | 1.91                     | 0.68              |
| 62:A5:1016:A:N7    | 62:A5:1106:A:N6    | 2.41                     | 0.68              |
| 69:AT:17:ALA:C     | 69:AT:21:PHE:CD2   | 2.70                     | 0.68              |
| 61:B2:1793:A:OP1   | 69:AT:91:HIS:NE2   | 2.27                     | 0.68              |
| 12:AS:117:ILE:HD12 | 17:AP:114:MET:HG2  | 1.76                     | 0.68              |
| 15:AL:144:LYS:HG2  | 15:AL:146:GLN:H    | 1.59                     | 0.68              |
| 61:B2:1109:C:O2'   | 61:B2:1213:A:N6    | 2.26                     | 0.68              |
| 61:B2:1660:U:O4'   | 69:AT:88:HIS:ND1   | 2.27                     | 0.68              |
| 61:B2:1715:G:C5    | 69:AT:67:ARG:HG2   | 2.28                     | 0.68              |
| 15:AL:129:ARG:HD2  | 61:B2:114:G:H5''   | 1.76                     | 0.67              |
| 62:A5:1121:A:H2    | 83:Cj:8:PHE:CE1    | 2.11                     | 0.67              |
| 61:B2:1715:G:O6    | 69:AT:67:ARG:HG3   | 1.90                     | 0.67              |
| 69:AT:129:ARG:HG2  | 69:AT:133:ARG:NE   | 2.06                     | 0.67              |
| 61:B2:578:A:H1'    | 61:B2:582:G:H22    | 1.60                     | 0.67              |
| 61:B2:1757:G:OP1   | 69:AT:38:LYS:NZ    | 2.28                     | 0.67              |
| 5:AC:115:ASP:HB3   | 5:AC:119:HIS:HB2   | 1.76                     | 0.67              |
| 21:Aa:88:SER:H     | 21:Aa:91:ALA:HB3   | 1.60                     | 0.67              |
| 59:A8:107:U:C6     | 83:Cj:20:ARG:HD2   | 2.16                     | 0.67              |
| 76:AQ:11:ALA:HB1   | 76:AQ:26:TYR:HB3   | 1.76                     | 0.67              |
| 8:AU:83:GLN:HG3    | 13:Ad:55:LEU:HB2   | 1.77                     | 0.67              |
| 27:Ca:35:ASN:HB2   | 62:A5:99:A:H5''    | 1.77                     | 0.67              |
| 2:CA:83:HIS:HB2    | 51:Cp:62:ARG:HD2   | 1.77                     | 0.67              |
| 61:B2:885:U:H2'    | 61:B2:886:G:H8     | 1.60                     | 0.67              |
| 62:A5:94:C:O2'     | 62:A5:300:A:OP1    | 2.13                     | 0.67              |
| 62:A5:2070:G:H1    | 62:A5:2082:U:H3    | 1.41                     | 0.67              |
| 69:AT:61:LEU:HD23  | 69:AT:132:ASP:OD2  | 1.91                     | 0.67              |
| 61:B2:148:G:N3     | 73:AG:13:GLN:NE2   | 2.43                     | 0.67              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 62:A5:3581:G:N2   | 62:A5:3582:A:N3    | 2.43                     | 0.67              |
| 61:B2:1693:C:OP1  | 69:AT:102:LYS:HE3  | 1.90                     | 0.67              |
| 62:A5:856:A:N7    | 62:A5:864:G:N2     | 2.42                     | 0.67              |
| 69:AT:42:PHE:HE1  | 69:AT:85:ASN:CG    | 2.01                     | 0.67              |
| 4:CB:243:LYS:NZ   | 62:A5:1074:U:OP2   | 2.27                     | 0.67              |
| 62:A5:1157:C:H42  | 62:A5:1165:A:H61   | 1.40                     | 0.67              |
| 62:A5:2839:A:H61  | 62:A5:2877:G:H21   | 1.43                     | 0.67              |
| 69:AT:59:SER:HB2  | 69:AT:63:HIS:NE2   | 2.08                     | 0.67              |
| 61:B2:1660:U:C1'  | 69:AT:88:HIS:CE1   | 2.78                     | 0.66              |
| 62:A5:173:A:N3    | 62:A5:274:A:N6     | 2.43                     | 0.66              |
| 62:A5:3407:U:OP2  | 62:A5:3476:G:N2    | 2.25                     | 0.66              |
| 75:AI:83:TYR:HB3  | 75:AI:101:ILE:HB   | 1.76                     | 0.66              |
| 76:AQ:49:LEU:HB3  | 76:AQ:87:ARG:HH22  | 1.59                     | 0.66              |
| 34:CT:12:ARG:NH2  | 62:A5:1263:U:OP2   | 2.29                     | 0.66              |
| 69:AT:54:TYR:CE1  | 69:AT:103:ALA:HB1  | 2.29                     | 0.66              |
| 4:CB:79:LEU:HD12  | 4:CB:333:ILE:HD11  | 1.75                     | 0.66              |
| 62:A5:1796:A:N6   | 62:A5:2551:U:OP2   | 2.28                     | 0.66              |
| 2:CA:124:GLY:O    | 2:CA:128:ARG:NH2   | 2.29                     | 0.66              |
| 61:B2:1717:A:C5'  | 69:AT:92:PHE:CE1   | 2.70                     | 0.66              |
| 61:B2:1727:U:C4   | 70:AF:190:ILE:CG1  | 2.78                     | 0.66              |
| 62:A5:214:A:N7    | 62:A5:241:C:N4     | 2.44                     | 0.66              |
| 23:AD:96:ARG:HG2  | 23:AD:103:GLN:HE22 | 1.60                     | 0.66              |
| 25:Af:139:HIS:H   | 25:Af:150:PHE:HB2  | 1.60                     | 0.66              |
| 38:CZ:134:ARG:NH2 | 62:A5:3001:A:O2'   | 2.29                     | 0.66              |
| 41:Cb:26:ARG:HG2  | 62:A5:1278:A:H61   | 1.59                     | 0.66              |
| 61:B2:1283:C:H41  | 76:AQ:147:TYR:HB2  | 1.61                     | 0.66              |
| 62:A5:789:G:O6    | 62:A5:800:C:N4     | 2.27                     | 0.66              |
| 69:AT:23:LYS:HG2  | 69:AT:28:LEU:HD23  | 1.77                     | 0.66              |
| 51:Cp:17:ARG:NH1  | 51:Cp:18:TYR:OH    | 2.29                     | 0.66              |
| 69:AT:75:ILE:C    | 69:AT:79:TYR:CE2   | 2.68                     | 0.66              |
| 19:AY:17:ARG:HH12 | 19:AY:78:ASP:HB3   | 1.59                     | 0.66              |
| 30:CD:22:ARG:HB3  | 30:CD:27:LYS:HB2   | 1.78                     | 0.66              |
| 35:CP:64:ASN:ND2  | 62:A5:2766:U:OP1   | 2.28                     | 0.66              |
| 62:A5:38:A:N7     | 62:A5:54:U:N3      | 2.43                     | 0.66              |
| 62:A5:3519:C:OP1  | 77:CO:67:ASN:ND2   | 2.25                     | 0.66              |
| 12:AS:39:ARG:HG2  | 69:AT:38:LYS:HZ2   | 0.66                     | 0.66              |
| 62:A5:1404:A:H3'  | 77:CO:51:ARG:HH21  | 1.61                     | 0.66              |
| 29:CI:151:ALA:HA  | 29:CI:154:ARG:HH21 | 1.62                     | 0.65              |
| 33:CS:116:ARG:NH1 | 62:A5:1426:U:O2'   | 2.29                     | 0.65              |
| 47:Ck:28:ASN:HB2  | 47:Ck:31:ASN:H     | 1.61                     | 0.65              |
| 62:A5:1031:G:O6   | 62:A5:1063:C:N4    | 2.28                     | 0.65              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 62:A5:1151:A:OP2  | 62:A5:1608:G:N2    | 2.29                     | 0.65              |
| 69:AT:75:ILE:HG22 | 69:AT:79:TYR:CD2   | 2.30                     | 0.65              |
| 6:CC:156:VAL:HG22 | 6:CC:255:TRP:HB2   | 1.79                     | 0.65              |
| 33:CS:15:ARG:HB3  | 33:CS:60:GLU:H     | 1.59                     | 0.65              |
| 59:A8:107:U:C5    | 83:Cj:20:ARG:HD3   | 2.25                     | 0.65              |
| 62:A5:1908:A:N7   | 62:A5:2133:A:N6    | 2.44                     | 0.65              |
| 62:A5:3859:C:N3   | 62:A5:3860:A:N6    | 2.44                     | 0.65              |
| 69:AT:17:ALA:CB   | 69:AT:21:PHE:HE2   | 2.09                     | 0.65              |
| 76:AQ:20:THR:HB   | 76:AQ:77:GLY:H     | 1.61                     | 0.65              |
| 23:AD:179:LEU:HG  | 23:AD:181:GLN:H    | 1.62                     | 0.65              |
| 62:A5:2161:G:C2'  | 83:Cj:5:THR:HG23   | 2.26                     | 0.65              |
| 62:A5:795:A:O2'   | 62:A5:797:A:OP2    | 2.14                     | 0.65              |
| 62:A5:1041:A:N6   | 62:A5:1052:U:O4    | 2.30                     | 0.65              |
| 69:AT:60:ILE:CG2  | 69:AT:64:LEU:HD12  | 2.27                     | 0.65              |
| 69:AT:60:ILE:HG22 | 69:AT:64:LEU:HD12  | 1.78                     | 0.65              |
| 6:CC:245:PRO:HB2  | 62:A5:1624:G:H4'   | 1.79                     | 0.65              |
| 62:A5:788:C:O2'   | 62:A5:1674:A:N6    | 2.29                     | 0.65              |
| 45:Cf:46:ARG:NH2  | 55:CE:234:SER:OG   | 2.28                     | 0.65              |
| 61:B2:132:A:H5'   | 61:B2:177:U:H5''   | 1.78                     | 0.65              |
| 61:B2:1671:U:C4   | 69:AT:82:ARG:CZ    | 2.79                     | 0.65              |
| 62:A5:58:G:N2     | 62:A5:60:G:O6      | 2.30                     | 0.65              |
| 62:A5:564:C:H42   | 62:A5:647:A:H61    | 1.42                     | 0.65              |
| 62:A5:797:A:O2'   | 62:A5:799:A:OP1    | 2.14                     | 0.65              |
| 6:CC:113:ARG:HA   | 28:CN:204:ARG:HH12 | 1.62                     | 0.65              |
| 33:CS:118:ARG:NH2 | 62:A5:1535:U:O2    | 2.29                     | 0.65              |
| 52:Co:44:LYS:O    | 52:Co:45:GLN:NE2   | 2.29                     | 0.65              |
| 20:AZ:48:LEU:HG   | 20:AZ:50:ASP:H     | 1.62                     | 0.65              |
| 35:CP:70:CYS:SG   | 35:CP:71:ALA:N     | 2.69                     | 0.65              |
| 52:Co:44:LYS:NZ   | 62:A5:96:G:OP1     | 2.28                     | 0.65              |
| 60:Cz:42:ASP:HB2  | 60:Cz:45:LYS:HE3   | 1.79                     | 0.65              |
| 61:B2:1734:G:H3'  | 69:AT:87:VAL:HG21  | 1.78                     | 0.65              |
| 7:Ag:11:LEU:HD21  | 7:Ag:53:TYR:H      | 1.62                     | 0.65              |
| 29:CI:160:PRO:O   | 29:CI:163:GLN:NE2  | 2.29                     | 0.65              |
| 62:A5:876:G:H1    | 62:A5:914:C:H42    | 1.44                     | 0.65              |
| 2:CA:174:ARG:NH2  | 62:A5:2558:A:OP1   | 2.29                     | 0.65              |
| 61:B2:1727:U:C2   | 70:AF:190:ILE:CB   | 2.80                     | 0.65              |
| 11:AM:98:LEU:HD13 | 11:AM:100:LYS:HZ3  | 1.61                     | 0.64              |
| 28:CN:153:LYS:NZ  | 62:A5:340:U:OP1    | 2.29                     | 0.64              |
| 62:A5:1643:G:H1   | 62:A5:1650:C:H42   | 1.44                     | 0.64              |
| 77:CO:16:HIS:HB3  | 77:CO:21:LEU:HD12  | 1.78                     | 0.64              |
| 44:Ce:123:ASN:ND2 | 62:A5:1652:U:O3'   | 2.31                     | 0.64              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 64:AW:78:ARG:HB3   | 64:AW:124:LYS:HD3  | 1.78                     | 0.64              |
| 69:AT:144:ASP:HA   | 69:AT:147:LYS:CG   | 2.27                     | 0.64              |
| 19:AY:64:ASN:HD21  | 61:B2:849:U:H5'    | 1.61                     | 0.64              |
| 28:CN:35:LYS:HB2   | 28:CN:65:ARG:HH21  | 1.61                     | 0.64              |
| 34:CT:37:GLY:HA2   | 34:CT:63:ARG:HD2   | 1.79                     | 0.64              |
| 35:CP:131:ARG:NH1  | 35:CP:137:ASN:OD1  | 2.31                     | 0.64              |
| 57:A9:12:C:H2'     | 57:A9:13:A:H8      | 1.60                     | 0.64              |
| 62:A5:1121:A:H2    | 83:Cj:8:PHE:CZ     | 2.14                     | 0.64              |
| 62:A5:1779:G:H1    | 62:A5:1869:C:H42   | 1.42                     | 0.64              |
| 62:A5:3644:C:N4    | 62:A5:3654:C:O2'   | 2.31                     | 0.64              |
| 6:CC:26:CYS:SG     | 6:CC:27:LEU:N      | 2.71                     | 0.64              |
| 8:AU:59:PRO:HG3    | 61:B2:1574:U:H4'   | 1.79                     | 0.64              |
| 27:Ca:25:LYS:NZ    | 62:A5:1142:U:O4    | 2.24                     | 0.64              |
| 44:Ce:21:ARG:O     | 44:Ce:24:SER:OG    | 2.13                     | 0.64              |
| 60:Cz:149:GLU:HA   | 60:Cz:152:LYS:HB3  | 1.78                     | 0.64              |
| 61:B2:50:C:OP1     | 61:B2:428:G:N2     | 2.30                     | 0.64              |
| 61:B2:1581:A:N6    | 61:B2:1605:G:N3    | 2.46                     | 0.64              |
| 5:AC:174:VAL:HG11  | 5:AC:219:PHE:HA    | 1.80                     | 0.64              |
| 61:B2:244:A:H62    | 61:B2:916:U:H3'    | 1.62                     | 0.64              |
| 62:A5:1016:A:P     | 83:Cj:28:HIS:HE2   | 2.18                     | 0.64              |
| 62:A5:1986:G:H1    | 62:A5:2086:U:H3    | 1.45                     | 0.64              |
| 66:Cg:2:VAL:HG21   | 66:Cg:30:LEU:HD21  | 1.79                     | 0.64              |
| 6:CC:226:ASN:ND2   | 62:A5:231:A:N3     | 2.45                     | 0.64              |
| 13:Ad:32:ARG:HH11  | 13:Ad:33:LYS:HG2   | 1.63                     | 0.64              |
| 15:AL:33:ARG:NH1   | 61:B2:213:G:N7     | 2.45                     | 0.64              |
| 45:Cf:49:ARG:NH1   | 62:A5:3714:U:OP1   | 2.31                     | 0.64              |
| 62:A5:3481:G:N1    | 62:A5:3510:U:O2'   | 2.30                     | 0.64              |
| 1:AA:163:CYS:SG    | 1:AA:164:ASN:N     | 2.70                     | 0.64              |
| 30:CD:33:ARG:NH1   | 58:A7:7:G:OP1      | 2.31                     | 0.64              |
| 48:Cl:8:ARG:NH2    | 83:Cj:20:ARG:HE    | 1.94                     | 0.64              |
| 13:Ad:17:GLY:HA2   | 13:Ad:27:ARG:HH12  | 1.63                     | 0.64              |
| 31:CQ:53:MET:HB2   | 31:CQ:58:ARG:HG3   | 1.79                     | 0.64              |
| 35:CP:65:GLY:HA2   | 35:CP:67:VAL:H     | 1.62                     | 0.64              |
| 39:Cr:95:LYS:HD2   | 55:CE:72:LYS:HG3   | 1.79                     | 0.64              |
| 61:B2:1316:G:N2    | 61:B2:1343:A:N7    | 2.46                     | 0.64              |
| 61:B2:1432:A:N7    | 61:B2:1435:A:N6    | 2.46                     | 0.64              |
| 79:CV:13:LYS:HG3   | 79:CV:128:LEU:HD11 | 1.79                     | 0.64              |
| 13:Ad:20:CYS:SG    | 13:Ad:27:ARG:NH1   | 2.71                     | 0.64              |
| 43:Cd:27:ALA:HA    | 43:Cd:30:VAL:HG12  | 1.79                     | 0.64              |
| 53:CJ:146:VAL:HG22 | 53:CJ:154:GLY:H    | 1.62                     | 0.64              |
| 62:A5:1698:A:OP1   | 62:A5:3613:G:N2    | 2.30                     | 0.64              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:Ag:196:LEU:HD21  | 7:Ag:210:SER:HB2   | 1.80                     | 0.64              |
| 17:AP:13:ARG:NH2   | 17:AP:18:PHE:O     | 2.31                     | 0.64              |
| 40:Ch:62:HIS:ND1   | 59:A8:95:A:OP1     | 2.30                     | 0.64              |
| 61:B2:1715:G:C5'   | 69:AT:78:ILE:HD12  | 2.23                     | 0.64              |
| 28:CN:188:ARG:NH1  | 62:A5:35:C:OP2     | 2.30                     | 0.63              |
| 62:A5:3732:U:H3    | 62:A5:3749:A:H61   | 1.46                     | 0.63              |
| 69:AT:20:VAL:O     | 69:AT:24:LYS:HG3   | 1.99                     | 0.63              |
| 69:AT:50:PRO:HD2   | 69:AT:51:ASP:H     | 1.63                     | 0.63              |
| 4:CB:215:GLU:HB2   | 4:CB:284:ILE:HD12  | 1.79                     | 0.63              |
| 5:AC:127:SER:HG    | 5:AC:132:THR:HG1   | 1.46                     | 0.63              |
| 62:A5:1644:C:N4    | 62:A5:1645:G:O6    | 2.31                     | 0.63              |
| 62:A5:1732:A:OP2   | 62:A5:2154:A:N6    | 2.31                     | 0.63              |
| 69:AT:29:LYS:CD    | 69:AT:106:ALA:N    | 2.62                     | 0.63              |
| 69:AT:61:LEU:HD22  | 69:AT:132:ASP:CG   | 2.13                     | 0.63              |
| 69:AT:71:GLY:O     | 69:AT:75:ILE:HG13  | 1.98                     | 0.63              |
| 30:CD:222:GLN:OE1  | 58:A7:30:G:N2      | 2.31                     | 0.63              |
| 59:A8:108:A:C8     | 83:Cj:29:LEU:CD2   | 2.81                     | 0.63              |
| 62:A5:126:G:H1     | 62:A5:157:C:H42    | 1.45                     | 0.63              |
| 62:A5:709:U:H2'    | 62:A5:710:A:H8     | 1.63                     | 0.63              |
| 62:A5:2101:C:H2'   | 62:A5:2102:G:H8    | 1.62                     | 0.63              |
| 62:A5:2168:G:N2    | 83:Cj:9:GLY:HA3    | 2.14                     | 0.63              |
| 69:AT:59:SER:CB    | 69:AT:63:HIS:CD2   | 2.79                     | 0.63              |
| 73:AG:57:ASP:HA    | 73:AG:107:SER:H    | 1.64                     | 0.63              |
| 22:Ab:17:ARG:HD3   | 61:B2:1157:C:H4'   | 1.80                     | 0.63              |
| 29:CI:196:ASN:H    | 29:CI:196:ASN:HD22 | 1.47                     | 0.63              |
| 46:CI:38:ARG:NH2   | 62:A5:333:C:OP2    | 2.32                     | 0.63              |
| 61:B2:561:G:H3'    | 61:B2:562:C:H2'    | 1.79                     | 0.63              |
| 12:AS:130:ARG:NH2  | 61:B2:1261:C:OP1   | 2.31                     | 0.63              |
| 28:CN:187:SER:OG   | 28:CN:188:ARG:N    | 2.25                     | 0.63              |
| 29:CI:33:ILE:O     | 29:CI:69:ARG:NH1   | 2.31                     | 0.63              |
| 39:Cr:74:ALA:O     | 39:Cr:83:ARG:NH2   | 2.31                     | 0.63              |
| 62:A5:1960:C:H42   | 62:A5:2120:G:H1    | 1.45                     | 0.63              |
| 69:AT:10:ASP:CG    | 76:AQ:43:GLN:O     | 2.41                     | 0.63              |
| 28:CN:172:ARG:NH2  | 62:A5:67:A:OP1     | 2.28                     | 0.63              |
| 45:Cf:68:GLU:OE2   | 62:A5:782:G:N2     | 2.28                     | 0.63              |
| 61:B2:1170:G:OP2   | 64:AW:20:ARG:NH1   | 2.31                     | 0.63              |
| 62:A5:1560:A:H2'   | 62:A5:1561:G:H8    | 1.63                     | 0.63              |
| 17:AP:46:ARG:NH2   | 61:B2:1744:U:OP2   | 2.32                     | 0.63              |
| 28:CN:143:ARG:HH22 | 62:A5:141:U:H3     | 1.46                     | 0.63              |
| 33:CS:174:THR:OG1  | 33:CS:175:TYR:N    | 2.32                     | 0.63              |
| 43:Cd:80:ARG:NH1   | 62:A5:3899:A:OP1   | 2.32                     | 0.63              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 61:B2:1209:U:H3    | 61:B2:1214:A:H61  | 1.46                     | 0.63              |
| 62:A5:546:G:H21    | 62:A5:3842:A:H2'  | 1.64                     | 0.63              |
| 62:A5:2014:C:H3'   | 62:A5:2015:G:H8   | 1.64                     | 0.63              |
| 62:A5:3495:G:H21   | 62:A5:3497:G:H8   | 1.45                     | 0.63              |
| 39:Cr:75:GLN:HE21  | 39:Cr:83:ARG:HE   | 1.46                     | 0.63              |
| 53:CJ:12:PRO:HD2   | 53:CJ:14:LYS:HB2  | 1.81                     | 0.63              |
| 61:B2:136:A:H62    | 61:B2:271:A:H61   | 1.46                     | 0.63              |
| 61:B2:1579:G:H3'   | 61:B2:1580:G:H8   | 1.64                     | 0.63              |
| 79:CV:66:LYS:O     | 79:CV:73:ARG:NH2  | 2.31                     | 0.63              |
| 15:AL:17:LEU:O     | 15:AL:19:ARG:NH1  | 2.32                     | 0.63              |
| 44:Ce:15:ARG:NH1   | 44:Ce:17:LYS:O    | 2.32                     | 0.63              |
| 62:A5:1702:G:H22   | 62:A5:1715:G:H1   | 1.45                     | 0.63              |
| 69:AT:136:ASN:C    | 69:AT:140:PHE:CD2 | 2.68                     | 0.63              |
| 75:AI:132:LYS:HD3  | 75:AI:135:GLU:HB3 | 1.79                     | 0.63              |
| 4:CB:117:ARG:NH1   | 62:A5:3887:U:OP1  | 2.32                     | 0.62              |
| 28:CN:12:ARG:HB2   | 28:CN:13:LYS:HE3  | 1.81                     | 0.62              |
| 45:Cf:119:GLY:HA3  | 45:Cf:135:PHE:HA  | 1.81                     | 0.62              |
| 53:CJ:92:LEU:HB3   | 53:CJ:97:TYR:HB3  | 1.80                     | 0.62              |
| 56:CG:83:PRO:HB3   | 56:CG:242:TRP:HB3 | 1.80                     | 0.62              |
| 61:B2:405:A:H62    | 75:AI:29:LEU:HD13 | 1.63                     | 0.62              |
| 62:A5:1533:A:OP1   | 77:CO:20:ARG:NH2  | 2.32                     | 0.62              |
| 62:A5:1930:G:H1    | 62:A5:1937:G:H1   | 1.47                     | 0.62              |
| 62:A5:3802:U:N3    | 77:CO:109:GLY:O   | 2.32                     | 0.62              |
| 30:CD:195:HIS:HA   | 30:CD:198:HIS:HB2 | 1.81                     | 0.62              |
| 59:A8:108:A:C8     | 83:Cj:29:LEU:HD22 | 2.33                     | 0.62              |
| 61:B2:274:G:N7     | 73:AG:188:ARG:NH1 | 2.47                     | 0.62              |
| 61:B2:1783:U:OP1   | 69:AT:92:PHE:CD2  | 2.53                     | 0.62              |
| 12:AS:35:GLY:O     | 12:AS:85:ASN:ND2  | 2.32                     | 0.62              |
| 40:Ch:109:ARG:HH12 | 62:A5:270:G:H4'   | 1.62                     | 0.62              |
| 41:Cb:6:ASN:O      | 41:Cb:8:THR:OG1   | 2.17                     | 0.62              |
| 62:A5:178:U:N3     | 62:A5:271:A:N1    | 2.47                     | 0.62              |
| 62:A5:1074:U:N3    | 62:A5:3509:U:OP1  | 2.32                     | 0.62              |
| 62:A5:1721:C:H42   | 62:A5:2191:G:H1   | 1.47                     | 0.62              |
| 78:CL:30:ARG:O     | 78:CL:34:ARG:NH1  | 2.33                     | 0.62              |
| 83:Cj:24:ASN:OD1   | 83:Cj:24:ASN:N    | 2.29                     | 0.62              |
| 56:CG:198:LEU:O    | 56:CG:200:ARG:NH1 | 2.33                     | 0.62              |
| 62:A5:439:U:O4     | 77:CO:98:GLN:NE2  | 2.31                     | 0.62              |
| 62:A5:1012:G:O6    | 62:A5:1128:C:N4   | 2.31                     | 0.62              |
| 2:CA:234:LYS:NZ    | 62:A5:2541:C:OP1  | 2.32                     | 0.62              |
| 13:Ad:12:ARG:HB2   | 13:Ad:18:SER:H    | 1.65                     | 0.62              |
| 61:B2:1601:A:N6    | 61:B2:1605:G:OP2  | 2.32                     | 0.62              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 61:B2:1715:G:H3'  | 69:AT:78:ILE:HG21  | 1.80                     | 0.62              |
| 61:B2:1727:U:N3   | 70:AF:190:ILE:CG1  | 2.62                     | 0.62              |
| 4:CB:261:ARG:HD2  | 62:A5:2744:C:H4'   | 1.80                     | 0.62              |
| 8:AU:83:GLN:HB2   | 13:Ad:55:LEU:HD23  | 1.81                     | 0.62              |
| 32:CR:106:LEU:O   | 32:CR:110:ARG:N    | 2.33                     | 0.62              |
| 44:Ce:34:TRP:O    | 44:Ce:35:ARG:NH1   | 2.30                     | 0.62              |
| 61:B2:1648:C:H5'' | 61:B2:1649:U:H5''  | 1.82                     | 0.62              |
| 62:A5:2239:C:N4   | 62:A5:2244:G:O6    | 2.32                     | 0.62              |
| 69:AT:85:ASN:ND2  | 69:AT:91:HIS:C     | 2.58                     | 0.62              |
| 26:AJ:29:GLU:HA   | 26:AJ:32:ILE:HD12  | 1.80                     | 0.62              |
| 39:Cr:101:LEU:O   | 39:Cr:105:LYS:NZ   | 2.31                     | 0.62              |
| 59:A8:58:C:N4     | 59:A8:97:U:O2'     | 2.30                     | 0.62              |
| 6:CC:5:ASN:ND2    | 62:A5:497:U:OP1    | 2.33                     | 0.62              |
| 30:CD:108:ARG:HE  | 30:CD:253:HIS:HA   | 1.65                     | 0.62              |
| 31:CQ:68:ARG:NH2  | 62:A5:870:U:O3'    | 2.32                     | 0.62              |
| 59:A8:40:A:N6     | 59:A8:100:G:O2'    | 2.33                     | 0.62              |
| 33:CS:86:SER:OG   | 62:A5:1510:G:OP1   | 2.18                     | 0.62              |
| 38:CZ:25:ILE:HA   | 38:CZ:43:VAL:HA    | 1.82                     | 0.62              |
| 62:A5:577:A:N1    | 62:A5:634:U:N3     | 2.47                     | 0.62              |
| 62:A5:641:A:N6    | 62:A5:644:U:O2     | 2.32                     | 0.62              |
| 62:A5:3924:U:O2'  | 62:A5:3925:G:N2    | 2.33                     | 0.62              |
| 19:AY:28:VAL:HB   | 19:AY:70:SER:HB2   | 1.82                     | 0.62              |
| 44:Ce:13:LYS:NZ   | 62:A5:1644:C:OP1   | 2.33                     | 0.62              |
| 62:A5:661:G:H2'   | 62:A5:662:A:H8     | 1.65                     | 0.62              |
| 62:A5:714:A:H2    | 62:A5:722:U:H3     | 1.47                     | 0.62              |
| 62:A5:2658:A:N6   | 62:A5:2688:U:O2'   | 2.32                     | 0.62              |
| 66:Cg:18:ASN:N    | 66:Cg:18:ASN:OD1   | 2.32                     | 0.62              |
| 70:AF:212:TYR:HB2 | 70:AF:214:ILE:HG22 | 1.81                     | 0.62              |
| 77:CO:18:LEU:HD11 | 77:CO:82:PHE:HA    | 1.81                     | 0.62              |
| 10:AX:26:ASP:O    | 10:AX:29:LYS:NZ    | 2.27                     | 0.61              |
| 32:CR:84:THR:HG22 | 62:A5:2231:A:H5''  | 1.82                     | 0.61              |
| 61:B2:1392:U:OP2  | 61:B2:1393:C:N4    | 2.33                     | 0.61              |
| 61:B2:1445:A:HO2' | 69:AT:133:ARG:NH1  | 1.97                     | 0.61              |
| 61:B2:1540:G:P    | 69:AT:7:LYS:NZ     | 2.73                     | 0.61              |
| 62:A5:2026:G:H21  | 62:A5:2044:A:H62   | 1.46                     | 0.61              |
| 69:AT:23:LYS:CG   | 69:AT:28:LEU:CD2   | 2.78                     | 0.61              |
| 3:AB:126:ALA:HB3  | 3:AB:142:CYS:HB2   | 1.82                     | 0.61              |
| 44:Ce:125:ASN:HA  | 44:Ce:128:LEU:HB2  | 1.81                     | 0.61              |
| 56:CG:108:ARG:HG2 | 56:CG:198:LEU:HD12 | 1.82                     | 0.61              |
| 61:B2:1540:G:N2   | 69:AT:129:ARG:NH2  | 2.38                     | 0.61              |
| 62:A5:2659:A:N6   | 62:A5:3490:C:O2'   | 2.33                     | 0.61              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 62:A5:3549:C:O2    | 62:A5:3576:G:N2    | 2.33                     | 0.61              |
| 73:AG:31:ARG:NH1   | 73:AG:100:CYS:SG   | 2.73                     | 0.61              |
| 4:CB:17:TYR:OH     | 4:CB:277:ARG:NH1   | 2.31                     | 0.61              |
| 4:CB:121:ASN:ND2   | 62:A5:3870:A:OP2   | 2.33                     | 0.61              |
| 28:CN:156:HIS:NE2  | 62:A5:340:U:OP2    | 2.33                     | 0.61              |
| 70:AF:121:PHE:HA   | 70:AF:124:ILE:HD12 | 1.82                     | 0.61              |
| 3:AB:35:ALA:O      | 3:AB:42:ARG:NH1    | 2.33                     | 0.61              |
| 3:AB:162:SER:HA    | 3:AB:165:ARG:HG2   | 1.82                     | 0.61              |
| 28:CN:113:LEU:HD22 | 28:CN:136:ASP:HA   | 1.80                     | 0.61              |
| 51:Cp:17:ARG:NH2   | 62:A5:1060:G:OP1   | 2.33                     | 0.61              |
| 62:A5:855:A:O4'    | 62:A5:865:A:N6     | 2.34                     | 0.61              |
| 62:A5:3591:A:H61   | 62:A5:3620:G:H3'   | 1.64                     | 0.61              |
| 64:AW:15:ASN:ND2   | 64:AW:72:CYS:O     | 2.33                     | 0.61              |
| 77:CO:126:MET:HB2  | 77:CO:129:LEU:HB2  | 1.83                     | 0.61              |
| 3:AB:137:LEU:HB2   | 3:AB:222:LYS:HB2   | 1.82                     | 0.61              |
| 4:CB:373:LYS:HE2   | 62:A5:3585:A:H4'   | 1.83                     | 0.61              |
| 10:AX:33:GLY:O     | 10:AX:37:LYS:NZ    | 2.34                     | 0.61              |
| 15:AL:71:THR:HA    | 15:AL:124:THR:HA   | 1.82                     | 0.61              |
| 28:CN:124:ASP:N    | 28:CN:124:ASP:OD1  | 2.31                     | 0.61              |
| 75:AI:151:TYR:HA   | 75:AI:154:ARG:HB2  | 1.81                     | 0.61              |
| 77:CO:94:THR:HG1   | 77:CO:97:GLY:H     | 1.45                     | 0.61              |
| 77:CO:192:GLU:O    | 77:CO:196:LYS:NZ   | 2.33                     | 0.61              |
| 51:Cp:51:VAL:HG12  | 51:Cp:52:VAL:HG23  | 1.83                     | 0.61              |
| 61:B2:1777:U:H3    | 61:B2:1803:A:H2    | 1.48                     | 0.61              |
| 62:A5:230:C:H2'    | 62:A5:231:A:H8     | 1.65                     | 0.61              |
| 62:A5:840:U:H1'    | 62:A5:841:A:H5'    | 1.82                     | 0.61              |
| 62:A5:1107:G:N2    | 62:A5:1125:A:O2'   | 2.34                     | 0.61              |
| 62:A5:1910:C:H1'   | 62:A5:2130:G:H5''  | 1.82                     | 0.61              |
| 75:AI:84:ASN:HA    | 75:AI:100:SER:HB2  | 1.83                     | 0.61              |
| 29:CI:111:LEU:HA   | 81:B:73:C:H1'      | 1.82                     | 0.61              |
| 58:A7:29:C:N3      | 58:A7:49:A:N6      | 2.48                     | 0.61              |
| 62:A5:2220:C:H4'   | 62:A5:3454:G:H5''  | 1.83                     | 0.61              |
| 62:A5:3567:A:H5'   | 62:A5:3568:A:H5''  | 1.83                     | 0.61              |
| 5:AC:208:SER:HB2   | 61:B2:3:U:H5''     | 1.82                     | 0.61              |
| 16:AR:71:ILE:HD13  | 16:AR:74:GLN:HG2   | 1.82                     | 0.61              |
| 19:AY:63:THR:HG1   | 19:AY:70:SER:HG    | 1.47                     | 0.61              |
| 24:Ae:103:ARG:NH2  | 61:B2:482:A:O2'    | 2.34                     | 0.61              |
| 52:Co:39:ARG:NH2   | 62:A5:302:A:OP2    | 2.33                     | 0.61              |
| 61:B2:1441:C:H42   | 61:B2:1543:G:H1    | 1.48                     | 0.61              |
| 62:A5:1895:U:H2'   | 62:A5:1896:A:H8    | 1.66                     | 0.61              |
| 83:Cj:45:ARG:NE    | 83:Cj:45:ARG:O     | 2.34                     | 0.61              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:CB:372:SER:OG    | 4:CB:373:LYS:N     | 2.33                     | 0.61              |
| 22:Ab:1:MET:HG2    | 22:Ab:3:LEU:H      | 1.65                     | 0.61              |
| 28:CN:9:GLU:OE1    | 46:Ci:51:ARG:NH1   | 2.33                     | 0.61              |
| 33:CS:150:ILE:HG13 | 33:CS:152:PHE:HB2  | 1.81                     | 0.61              |
| 39:Cr:96:LYS:NZ    | 62:A5:476:U:O4     | 2.34                     | 0.61              |
| 61:B2:1301:G:O2'   | 61:B2:1331:A:N6    | 2.31                     | 0.61              |
| 61:B2:1671:U:O4    | 69:AT:82:ARG:NE    | 2.33                     | 0.61              |
| 61:B2:1693:C:OP1   | 69:AT:102:LYS:NZ   | 2.34                     | 0.61              |
| 62:A5:988:C:H2'    | 62:A5:989:A:H8     | 1.66                     | 0.61              |
| 63:Ac:38:ILE:HD13  | 63:Ac:40:ARG:HH21  | 1.66                     | 0.61              |
| 9:AO:146:ARG:NH2   | 61:B2:1984:G:OP2   | 2.30                     | 0.61              |
| 10:AX:8:ARG:NH1    | 61:B2:641:U:OP2    | 2.34                     | 0.61              |
| 19:AY:25:VAL:HA    | 19:AY:73:PHE:HA    | 1.82                     | 0.61              |
| 25:Af:79:LYS:H     | 61:B2:1639:U:H5    | 1.48                     | 0.61              |
| 30:CD:10:LYS:HD3   | 30:CD:11:GLN:HG3   | 1.81                     | 0.61              |
| 56:CG:202:LYS:NZ   | 62:A5:153:G:OP2    | 2.34                     | 0.61              |
| 61:B2:1660:U:H1'   | 69:AT:88:HIS:HE1   | 1.65                     | 0.61              |
| 78:CL:168:GLU:HG2  | 78:CL:170:THR:HG23 | 1.83                     | 0.61              |
| 78:CL:186:ARG:NH1  | 78:CL:186:ARG:O    | 2.33                     | 0.61              |
| 10:AX:133:LEU:O    | 10:AX:140:ARG:NH1  | 2.34                     | 0.60              |
| 17:AP:8:ASN:HD22   | 17:AP:8:ASN:N      | 1.97                     | 0.60              |
| 27:Ca:13:ARG:NH2   | 62:A5:811:G:OP2    | 2.34                     | 0.60              |
| 32:CR:120:TYR:O    | 32:CR:124:TYR:N    | 2.34                     | 0.60              |
| 33:CS:83:ARG:NH2   | 34:CT:155:TYR:O    | 2.34                     | 0.60              |
| 39:Cr:43:ARG:HE    | 39:Cr:48:VAL:HG21  | 1.66                     | 0.60              |
| 52:Co:59:LYS:NZ    | 62:A5:3326:G:OP1   | 2.34                     | 0.60              |
| 59:A8:108:A:N7     | 83:Cj:29:LEU:HD22  | 2.16                     | 0.60              |
| 62:A5:1994:U:H3    | 67:CU:261:ARG:HD2  | 1.66                     | 0.60              |
| 62:A5:3231:G:H1    | 62:A5:3287:C:H42   | 1.47                     | 0.60              |
| 69:AT:18:VAL:CA    | 69:AT:21:PHE:HD2   | 2.12                     | 0.60              |
| 1:AA:185:LEU:HD11  | 18:AV:39:VAL:HG13  | 1.82                     | 0.60              |
| 6:CC:321:PRO:HG3   | 71:CF:158:TYR:HB3  | 1.83                     | 0.60              |
| 44:Ce:15:ARG:NH2   | 62:A5:446:C:OP1    | 2.32                     | 0.60              |
| 52:Co:3:ASN:HB2    | 62:A5:3187:C:H3'   | 1.83                     | 0.60              |
| 55:CE:78:ARG:NH2   | 62:A5:460:A:OP1    | 2.34                     | 0.60              |
| 62:A5:1121:A:C2    | 83:Cj:8:PHE:CE1    | 2.89                     | 0.60              |
| 66:Cg:81:CYS:N     | 66:Cg:84:CYS:SG    | 2.69                     | 0.60              |
| 79:CV:13:LYS:HB2   | 79:CV:128:LEU:HD21 | 1.82                     | 0.60              |
| 2:CA:190:LYS:HG2   | 2:CA:191:VAL:HG13  | 1.83                     | 0.60              |
| 8:AU:64:ARG:NH2    | 61:B2:1797:G:O2'   | 2.34                     | 0.60              |
| 28:CN:68:ARG:NE    | 62:A5:309:C:OP1    | 2.33                     | 0.60              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 62:A5:1398:C:H2'   | 62:A5:1399:A:C8    | 2.36                     | 0.60              |
| 8:AU:25:THR:HG1    | 8:AU:88:LYS:HZ1    | 1.48                     | 0.60              |
| 19:AY:22:LYS:HB2   | 19:AY:76:ILE:HB    | 1.83                     | 0.60              |
| 33:CS:43:ARG:NH2   | 58:A7:95:U:OP1     | 2.34                     | 0.60              |
| 62:A5:2644:U:HO2'  | 81:B:12:G:HO2'     | 1.48                     | 0.60              |
| 62:A5:3725:U:OP2   | 77:CO:14:ARG:NH2   | 2.35                     | 0.60              |
| 67:CU:194:VAL:O    | 67:CU:245:HIS:ND1  | 2.34                     | 0.60              |
| 69:AT:29:LYS:HZ2   | 69:AT:106:ALA:CA   | 1.98                     | 0.60              |
| 2:CA:67:TYR:OH     | 62:A5:2919:A:N7    | 2.31                     | 0.60              |
| 4:CB:378:ARG:NH2   | 62:A5:3905:U:OP2   | 2.34                     | 0.60              |
| 9:AO:55:ARG:HE     | 61:B2:984:G:H21    | 1.50                     | 0.60              |
| 9:AO:75:MET:HB2    | 63:Ac:59:ARG:HH12  | 1.65                     | 0.60              |
| 16:AR:92:GLU:HG3   | 16:AR:96:ILE:HG12  | 1.82                     | 0.60              |
| 26:AJ:72:LEU:O     | 26:AJ:76:ASN:ND2   | 2.33                     | 0.60              |
| 29:CI:71:CYS:SG    | 29:CI:158:LYS:NZ   | 2.72                     | 0.60              |
| 33:CS:101:THR:HG23 | 33:CS:104:GLY:H    | 1.66                     | 0.60              |
| 34:CT:130:ARG:NH1  | 62:A5:1311:U:OP1   | 2.34                     | 0.60              |
| 46:Ci:75:LYS:HE3   | 46:Ci:78:ARG:HD2   | 1.84                     | 0.60              |
| 49:Cm:93:LYS:NZ    | 62:A5:3643:C:OP1   | 2.35                     | 0.60              |
| 61:B2:1445:A:H4'   | 69:AT:133:ARG:CZ   | 2.31                     | 0.60              |
| 61:B2:1540:G:N2    | 69:AT:129:ARG:HE   | 1.98                     | 0.60              |
| 62:A5:473:A:N6     | 62:A5:527:U:O4     | 2.33                     | 0.60              |
| 5:AC:54:ARG:NH2    | 5:AC:75:GLU:OE1    | 2.34                     | 0.60              |
| 6:CC:226:ASN:O     | 62:A5:234:G:O2'    | 2.20                     | 0.60              |
| 32:CR:5:LYS:NZ     | 62:A5:1756:G:OP1   | 2.34                     | 0.60              |
| 35:CP:62:ARG:NH2   | 62:A5:430:G:OP1    | 2.34                     | 0.60              |
| 37:CY:2:LYS:NZ     | 62:A5:234:G:OP2    | 2.35                     | 0.60              |
| 72:AE:48:LEU:HA    | 72:AE:52:LEU:HB2   | 1.83                     | 0.60              |
| 75:AI:73:ALA:O     | 75:AI:74:ARG:NH1   | 2.35                     | 0.60              |
| 2:CA:30:ARG:O      | 2:CA:163:ARG:NH2   | 2.35                     | 0.60              |
| 28:CN:138:HIS:NE2  | 40:Ch:93:LYS:O     | 2.34                     | 0.60              |
| 35:CP:45:GLN:NE2   | 35:CP:99:GLU:OE1   | 2.35                     | 0.60              |
| 42:Cc:46:VAL:HB    | 42:Cc:71:VAL:HG12  | 1.83                     | 0.60              |
| 44:Ce:113:ARG:HE   | 44:Ce:117:LEU:HD11 | 1.67                     | 0.60              |
| 51:Cp:49:ARG:NH2   | 62:A5:2106:C:OP2   | 2.34                     | 0.60              |
| 58:A7:84:U:O4      | 62:A5:1412:A:N6    | 2.34                     | 0.60              |
| 61:B2:451:C:OP1    | 72:AE:57:ASN:ND2   | 2.34                     | 0.60              |
| 61:B2:1063:G:H1    | 61:B2:1110:A:HO2'  | 1.48                     | 0.60              |
| 61:B2:1831:C:H42   | 61:B2:1958:A:H61   | 1.49                     | 0.60              |
| 62:A5:78:A:O2'     | 78:CL:59:ARG:O     | 2.16                     | 0.60              |
| 62:A5:2065:A:H3'   | 62:A5:2066:G:C8    | 2.37                     | 0.60              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 71:CF:102:ASN:N    | 71:CF:102:ASN:OD1  | 2.35                     | 0.60              |
| 78:CL:79:GLU:HG2   | 78:CL:109:ARG:HG3  | 1.82                     | 0.60              |
| 3:AB:68:GLU:HG3    | 3:AB:86:LYS:HD2    | 1.82                     | 0.60              |
| 16:AR:28:PHE:H     | 61:B2:1584:A:H2    | 1.49                     | 0.60              |
| 30:CD:30:TYR:OH    | 58:A7:10:C:N4      | 2.34                     | 0.60              |
| 62:A5:1199:C:H42   | 62:A5:1311:U:H3    | 1.47                     | 0.60              |
| 62:A5:3700:U:H3    | 62:A5:3862:A:H1'   | 1.67                     | 0.60              |
| 7:Ag:171:TRP:O     | 16:AR:23:ARG:NH1   | 2.34                     | 0.60              |
| 29:CI:196:ASN:HD22 | 29:CI:196:ASN:N    | 1.99                     | 0.60              |
| 59:A8:107:U:C4     | 83:Cj:20:ARG:CD    | 2.83                     | 0.60              |
| 61:B2:67:A:N6      | 61:B2:82:G:O2'     | 2.33                     | 0.60              |
| 61:B2:872:A:N7     | 72:AE:108:ARG:NH1  | 2.50                     | 0.60              |
| 61:B2:1670:G:O6    | 61:B2:1720:A:N6    | 2.35                     | 0.60              |
| 62:A5:1015:G:O2'   | 62:A5:1120:A:N6    | 2.35                     | 0.60              |
| 62:A5:1805:A:C5    | 62:A5:1806:G:H1'   | 2.37                     | 0.60              |
| 62:A5:3699:U:H3    | 62:A5:3863:G:H22   | 1.47                     | 0.60              |
| 72:AE:9:LEU:HB2    | 72:AE:30:ARG:HH11  | 1.67                     | 0.60              |
| 4:CB:57:VAL:HG22   | 4:CB:73:VAL:HG12   | 1.84                     | 0.60              |
| 12:AS:83:PHE:CE2   | 69:AT:36:ILE:HG23  | 2.31                     | 0.60              |
| 47:Ck:24:LYS:HB2   | 47:Ck:35:LYS:HB2   | 1.84                     | 0.60              |
| 59:A8:41:G:N2      | 59:A8:42:A:N3      | 2.50                     | 0.60              |
| 61:B2:334:G:H5''   | 75:AI:98:LYS:HB3   | 1.83                     | 0.60              |
| 28:CN:69:GLY:O     | 62:A5:308:G:O2'    | 2.20                     | 0.59              |
| 56:CG:78:ARG:NH1   | 56:CG:247:LEU:O    | 2.35                     | 0.59              |
| 70:AF:132:PRO:HA   | 70:AF:135:ILE:HD12 | 1.84                     | 0.59              |
| 14:AN:71:ILE:HD13  | 61:B2:1048:U:H5''  | 1.84                     | 0.59              |
| 45:Cf:125:HIS:HB2  | 45:Cf:132:ARG:HE   | 1.66                     | 0.59              |
| 61:B2:127:U:H5''   | 61:B2:176:U:H5'    | 1.83                     | 0.59              |
| 62:A5:94:C:OP2     | 62:A5:97:C:N4      | 2.34                     | 0.59              |
| 62:A5:2630:A:H61   | 62:A5:2642:U:H3    | 1.50                     | 0.59              |
| 62:A5:3464:G:H2'   | 62:A5:3466:A:H5''  | 1.83                     | 0.59              |
| 1:AA:38:VAL:HA     | 1:AA:49:LEU:HA     | 1.83                     | 0.59              |
| 1:AA:149:ASN:ND2   | 1:AA:164:ASN:O     | 2.36                     | 0.59              |
| 5:AC:177:ARG:HH22  | 61:B2:615:G:H1     | 1.50                     | 0.59              |
| 39:Cr:13:ARG:NE    | 62:A5:1595:G:O2'   | 2.36                     | 0.59              |
| 55:CE:59:LYS:HB3   | 55:CE:63:LYS:HD3   | 1.84                     | 0.59              |
| 58:A7:74:A:N6      | 58:A7:101:A:OP2    | 2.36                     | 0.59              |
| 61:B2:1168:C:O2'   | 61:B2:1170:G:OP1   | 2.17                     | 0.59              |
| 62:A5:677:G:H1     | 62:A5:744:U:H3     | 1.50                     | 0.59              |
| 62:A5:1398:C:OP1   | 80:CM:51:ARG:NH1   | 2.35                     | 0.59              |
| 62:A5:2234:C:H42   | 62:A5:2250:G:H1    | 1.50                     | 0.59              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 62:A5:3544:G:H5'   | 77:CO:63:ARG:HH12 | 1.68                     | 0.59              |
| 69:AT:136:ASN:O    | 69:AT:140:PHE:CE2 | 2.51                     | 0.59              |
| 83:Cj:19:CYS:SG    | 83:Cj:20:ARG:N    | 2.74                     | 0.59              |
| 1:AA:6:ASP:N       | 1:AA:9:SER:HG     | 1.99                     | 0.59              |
| 25:Af:89:LYS:HG3   | 25:Af:91:ILE:HG12 | 1.83                     | 0.59              |
| 31:CQ:35:LEU:O     | 31:CQ:44:ASN:ND2  | 2.35                     | 0.59              |
| 36:CX:160:LYS:NZ   | 36:CX:161:ILE:O   | 2.36                     | 0.59              |
| 38:CZ:100:LEU:O    | 38:CZ:106:ARG:NH2 | 2.32                     | 0.59              |
| 39:Cr:93:SER:HB3   | 39:Cr:97:LEU:HB3  | 1.83                     | 0.59              |
| 45:Cf:74:LYS:NZ    | 77:CO:31:GLN:OE1  | 2.31                     | 0.59              |
| 61:B2:554:U:O4     | 61:B2:599:A:N6    | 2.35                     | 0.59              |
| 62:A5:1811:A:N6    | 62:A5:1860:A:OP1  | 2.36                     | 0.59              |
| 62:A5:1875:G:O2'   | 62:A5:2112:A:N1   | 2.36                     | 0.59              |
| 62:A5:3159:C:O2'   | 62:A5:3330:C:OP2  | 2.20                     | 0.59              |
| 62:A5:3688:A:O2'   | 62:A5:3690:A:N6   | 2.33                     | 0.59              |
| 7:Ag:291:ALA:HB3   | 7:Ag:300:PHE:HB2  | 1.82                     | 0.59              |
| 15:AL:19:ARG:NH2   | 75:AI:193:GLU:OE1 | 2.36                     | 0.59              |
| 23:AD:139:VAL:HG12 | 23:AD:153:LYS:HA  | 1.83                     | 0.59              |
| 61:B2:1137:G:O2'   | 61:B2:1139:A:N6   | 2.34                     | 0.59              |
| 62:A5:1909:U:O2    | 62:A5:2132:A:N6   | 2.28                     | 0.59              |
| 62:A5:2160:C:C1'   | 83:Cj:8:PHE:O     | 2.44                     | 0.59              |
| 62:A5:2824:U:O2    | 62:A5:2895:U:N3   | 2.34                     | 0.59              |
| 63:Ac:34:GLN:O     | 63:Ac:37:GLN:NE2  | 2.36                     | 0.59              |
| 69:AT:144:ASP:HA   | 69:AT:147:LYS:HG3 | 1.84                     | 0.59              |
| 76:AQ:36:VAL:HA    | 76:AQ:72:VAL:HB   | 1.84                     | 0.59              |
| 8:AU:75:GLY:H      | 8:AU:77:LYS:HG2   | 1.67                     | 0.59              |
| 12:AS:39:ARG:CG    | 69:AT:38:LYS:CE   | 2.78                     | 0.59              |
| 14:AN:10:GLY:HA3   | 61:B2:1042:A:H5'' | 1.84                     | 0.59              |
| 29:CI:107:GLY:O    | 29:CI:110:ARG:NH1 | 2.36                     | 0.59              |
| 31:CQ:91:ARG:NH1   | 62:A5:985:G:N7    | 2.51                     | 0.59              |
| 32:CR:72:LYS:O     | 32:CR:74:ARG:NH1  | 2.36                     | 0.59              |
| 45:Cf:113:ARG:NH1  | 62:A5:3706:U:OP1  | 2.35                     | 0.59              |
| 61:B2:1695:A:H5''  | 69:AT:33:GLN:CD   | 2.27                     | 0.59              |
| 62:A5:1584:A:H5'   | 71:CF:29:ILE:HB   | 1.85                     | 0.59              |
| 15:AL:74:VAL:HA    | 15:AL:85:ILE:HA   | 1.85                     | 0.59              |
| 20:AZ:48:LEU:HD23  | 20:AZ:77:LYS:HD3  | 1.83                     | 0.59              |
| 30:CD:52:ILE:HB    | 30:CD:63:GLN:HB2  | 1.82                     | 0.59              |
| 36:CX:243:ALA:HB3  | 36:CX:260:ARG:HB3 | 1.85                     | 0.59              |
| 45:Cf:134:ARG:NH1  | 62:A5:1379:U:OP1  | 2.36                     | 0.59              |
| 61:B2:157:C:OP1    | 73:AG:87:ARG:NH2  | 2.36                     | 0.59              |
| 61:B2:1671:U:H3    | 69:AT:82:ARG:CZ   | 2.15                     | 0.59              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 62:A5:291:U:H2'   | 62:A5:292:G:H8    | 1.68                     | 0.59              |
| 62:A5:1267:A:H5'' | 62:A5:3169:A:H61  | 1.68                     | 0.59              |
| 62:A5:1584:A:OP2  | 71:CF:32:ARG:NH2  | 2.34                     | 0.59              |
| 62:A5:1595:G:OP1  | 62:A5:1598:A:O2'  | 2.16                     | 0.59              |
| 69:AT:139:VAL:O   | 69:AT:143:ARG:HG3 | 2.02                     | 0.59              |
| 6:CC:289:ASN:N    | 31:CQ:124:ASP:OD2 | 2.35                     | 0.59              |
| 9:AO:101:GLY:HA2  | 9:AO:104:LYS:HB2  | 1.84                     | 0.59              |
| 34:CT:108:ARG:NH2 | 34:CT:128:LEU:O   | 2.35                     | 0.59              |
| 35:CP:21:ASN:OD1  | 35:CP:145:HIS:NE2 | 2.32                     | 0.59              |
| 45:Cf:110:ARG:NH2 | 62:A5:3845:A:O2'  | 2.36                     | 0.59              |
| 62:A5:918:G:H1    | 62:A5:982:C:H42   | 1.49                     | 0.59              |
| 62:A5:2160:C:H42  | 62:A5:2167:G:H1   | 1.49                     | 0.59              |
| 62:A5:2673:A:H1'  | 79:CV:40:ILE:HD11 | 1.85                     | 0.59              |
| 78:CL:46:PHE:HB3  | 78:CL:48:ARG:H    | 1.67                     | 0.59              |
| 2:CA:195:SER:OG   | 2:CA:196:TRP:N    | 2.35                     | 0.59              |
| 6:CC:314:ARG:NH1  | 62:A5:751:A:OP2   | 2.36                     | 0.59              |
| 8:AU:52:VAL:HG13  | 8:AU:91:ILE:HG23  | 1.85                     | 0.59              |
| 27:Ca:52:GLY:O    | 31:CQ:177:ALA:N   | 2.36                     | 0.59              |
| 34:CT:77:ASN:ND2  | 62:A5:1273:U:OP1  | 2.30                     | 0.59              |
| 61:B2:67:A:O2'    | 61:B2:69:A:N7     | 2.31                     | 0.59              |
| 61:B2:987:A:H3'   | 61:B2:988:G:H21   | 1.67                     | 0.59              |
| 61:B2:1354:G:HO2' | 61:B2:1640:G:HO2' | 1.51                     | 0.59              |
| 61:B2:1589:C:O2   | 61:B2:1590:G:N2   | 2.35                     | 0.59              |
| 62:A5:487:A:H61   | 62:A5:513:G:H1    | 1.50                     | 0.59              |
| 62:A5:2743:C:O2'  | 77:CO:70:ARG:NH1  | 2.35                     | 0.59              |
| 3:AB:161:GLN:O    | 3:AB:165:ARG:NE   | 2.34                     | 0.59              |
| 6:CC:174:LEU:HD22 | 6:CC:179:ILE:HD11 | 1.85                     | 0.59              |
| 12:AS:120:HIS:O   | 12:AS:124:ARG:NH1 | 2.36                     | 0.59              |
| 28:CN:44:ARG:HD3  | 28:CN:47:LYS:HB2  | 1.84                     | 0.59              |
| 30:CD:221:ARG:NH1 | 58:A7:30:G:O2'    | 2.35                     | 0.59              |
| 36:CX:231:ARG:NH2 | 62:A5:2145:G:OP1  | 2.36                     | 0.59              |
| 51:Cp:23:ARG:NH2  | 62:A5:2241:U:O2'  | 2.36                     | 0.59              |
| 55:CE:57:LYS:NZ   | 62:A5:1588:A:N3   | 2.50                     | 0.59              |
| 61:B2:521:U:N3    | 61:B2:522:G:O6    | 2.35                     | 0.59              |
| 61:B2:1853:U:OP1  | 79:CV:69:LYS:NZ   | 2.36                     | 0.59              |
| 75:AI:120:PRO:O   | 75:AI:123:ARG:NH1 | 2.36                     | 0.59              |
| 35:CP:84:PRO:HB2  | 35:CP:87:SER:HB2  | 1.84                     | 0.58              |
| 48:Cl:21:ARG:NH2  | 59:A8:51:A:OP1    | 2.35                     | 0.58              |
| 54:CH:87:GLN:NE2  | 54:CH:184:THR:O   | 2.36                     | 0.58              |
| 61:B2:1589:C:O2'  | 61:B2:1590:G:N3   | 2.34                     | 0.58              |
| 61:B2:1713:C:N4   | 69:AT:66:HIS:O    | 2.36                     | 0.58              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 62:A5:459:U:O3'    | 62:A5:541:A:N6     | 2.36                     | 0.58              |
| 62:A5:1473:U:O2'   | 62:A5:1475:A:N7    | 2.35                     | 0.58              |
| 62:A5:3791:A:H62   | 80:CM:144:LYS:HE2  | 1.68                     | 0.58              |
| 66:Cg:6:THR:OG1    | 66:Cg:7:LEU:N      | 2.32                     | 0.58              |
| 69:AT:80:GLY:O     | 69:AT:83:LYS:HE3   | 2.04                     | 0.58              |
| 15:AL:122:ILE:H    | 15:AL:145:GLY:HA2  | 1.67                     | 0.58              |
| 22:Ab:23:ARG:HH22  | 74:AH:194:VAL:HG12 | 1.68                     | 0.58              |
| 27:Ca:48:LYS:NZ    | 62:A5:1167:A:OP1   | 2.36                     | 0.58              |
| 33:CS:172:PRO:HD2  | 77:CO:126:MET:HE2  | 1.85                     | 0.58              |
| 46:Ci:55:ARG:HA    | 46:Ci:58:VAL:HG12  | 1.85                     | 0.58              |
| 61:B2:909:U:H3     | 61:B2:935:A:HO2'   | 1.50                     | 0.58              |
| 61:B2:1062:C:H2'   | 61:B2:1063:G:H8    | 1.68                     | 0.58              |
| 62:A5:56:A:C5'     | 83:Cj:48:ASN:CB    | 2.79                     | 0.58              |
| 62:A5:389:G:O2'    | 62:A5:413:A:N6     | 2.36                     | 0.58              |
| 62:A5:990:U:H2'    | 62:A5:991:A:C8     | 2.38                     | 0.58              |
| 62:A5:2781:G:O2'   | 62:A5:2784:C:N4    | 2.36                     | 0.58              |
| 77:CO:92:HIS:O     | 77:CO:98:GLN:NE2   | 2.36                     | 0.58              |
| 77:CO:197:ILE:HD12 | 77:CO:200:SER:HB2  | 1.85                     | 0.58              |
| 3:AB:154:ARG:NH1   | 61:B2:1132:U:OP1   | 2.37                     | 0.58              |
| 6:CC:199:MET:HE3   | 59:A8:20:C:H5''    | 1.84                     | 0.58              |
| 21:Aa:33:ASP:OD1   | 21:Aa:33:ASP:N     | 2.36                     | 0.58              |
| 22:Ab:23:ARG:NH1   | 22:Ab:27:HIS:O     | 2.36                     | 0.58              |
| 30:CD:215:ASP:HB3  | 30:CD:217:GLU:HG2  | 1.85                     | 0.58              |
| 32:CR:96:MET:SD    | 32:CR:100:ARG:NH2  | 2.75                     | 0.58              |
| 48:Cl:10:LYS:NZ    | 62:A5:2149:G:OP1   | 2.35                     | 0.58              |
| 61:B2:1144:C:N4    | 61:B2:1148:U:OP2   | 2.37                     | 0.58              |
| 61:B2:1672:A:O4'   | 69:AT:12:HIS:CE1   | 2.57                     | 0.58              |
| 61:B2:1982:C:H2'   | 61:B2:1983:G:H8    | 1.69                     | 0.58              |
| 62:A5:760:G:N2     | 62:A5:761:C:O2'    | 2.36                     | 0.58              |
| 62:A5:1326:A:N3    | 62:A5:1611:G:O2'   | 2.36                     | 0.58              |
| 62:A5:3183:G:N3    | 62:A5:3292:C:N4    | 2.51                     | 0.58              |
| 21:Aa:28:ARG:NH2   | 61:B2:1966:U:O4    | 2.36                     | 0.58              |
| 32:CR:110:ARG:NH1  | 62:A5:2032:U:OP1   | 2.36                     | 0.58              |
| 61:B2:137:C:H1'    | 61:B2:138:U:H4'    | 1.86                     | 0.58              |
| 61:B2:356:C:N4     | 61:B2:639:G:OP1    | 2.36                     | 0.58              |
| 61:B2:409:G:H22    | 73:AG:92:ARG:HH21  | 1.51                     | 0.58              |
| 61:B2:1667:A:C5'   | 69:AT:84:ARG:NH1   | 2.48                     | 0.58              |
| 61:B2:1783:U:OP1   | 69:AT:92:PHE:HD2   | 1.85                     | 0.58              |
| 61:B2:1786:G:H1    | 61:B2:1794:C:H42   | 1.50                     | 0.58              |
| 62:A5:480:C:H2'    | 62:A5:520:G:H22    | 1.68                     | 0.58              |
| 62:A5:1181:A:H1'   | 62:A5:1182:A:H5''  | 1.84                     | 0.58              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 62:A5:3408:C:O2    | 62:A5:3483:G:N1    | 2.35                     | 0.58              |
| 62:A5:3655:U:N3    | 62:A5:3658:G:N7    | 2.45                     | 0.58              |
| 62:A5:3729:A:OP1   | 62:A5:3730:G:N2    | 2.37                     | 0.58              |
| 74:AH:110:LEU:HG   | 74:AH:111:LYS:HD2  | 1.84                     | 0.58              |
| 77:CO:172:HIS:ND1  | 77:CO:173:ASN:OD1  | 2.36                     | 0.58              |
| 4:CB:21:ARG:HE     | 4:CB:271:GLN:HE21  | 1.51                     | 0.58              |
| 12:AS:142:ARG:HH12 | 61:B2:1259:A:H5''  | 1.68                     | 0.58              |
| 61:B2:1426:A:N7    | 61:B2:1579:G:N2    | 2.51                     | 0.58              |
| 62:A5:1645:G:H21   | 62:A5:1647:A:P     | 2.27                     | 0.58              |
| 75:AI:110:ARG:NH2  | 75:AI:168:PHE:O    | 2.36                     | 0.58              |
| 77:CO:94:THR:O     | 77:CO:98:GLN:NE2   | 2.37                     | 0.58              |
| 2:CA:143:THR:O     | 2:CA:145:LYS:NZ    | 2.31                     | 0.58              |
| 6:CC:47:LEU:HD12   | 6:CC:118:VAL:HG11  | 1.85                     | 0.58              |
| 29:CI:52:LEU:HD22  | 29:CI:152:LEU:HD22 | 1.85                     | 0.58              |
| 32:CR:166:VAL:HA   | 32:CR:169:ALA:HB3  | 1.85                     | 0.58              |
| 40:Ch:75:ASN:OD1   | 62:A5:138:A:N6     | 2.36                     | 0.58              |
| 45:Cf:81:LYS:NZ    | 62:A5:1542:C:OP1   | 2.37                     | 0.58              |
| 54:CH:31:ARG:NH1   | 54:CH:84:PHE:O     | 2.37                     | 0.58              |
| 61:B2:1695:A:C5'   | 69:AT:33:GLN:OE1   | 2.51                     | 0.58              |
| 71:CF:116:ARG:NH2  | 71:CF:209:SER:O    | 2.35                     | 0.58              |
| 5:AC:114:GLY:HA3   | 5:AC:120:ILE:HD12  | 1.86                     | 0.58              |
| 6:CC:237:LYS:NZ    | 62:A5:839:A:N7     | 2.52                     | 0.58              |
| 12:AS:13:LEU:HB2   | 12:AS:20:ILE:HB    | 1.86                     | 0.58              |
| 27:Ca:73:GLU:OE2   | 62:A5:864:G:N1     | 2.30                     | 0.58              |
| 28:CN:183:THR:HB   | 28:CN:188:ARG:HA   | 1.86                     | 0.58              |
| 29:CI:99:ILE:O     | 29:CI:121:LYS:N    | 2.36                     | 0.58              |
| 61:B2:239:G:N2     | 61:B2:240:U:O4     | 2.36                     | 0.58              |
| 61:B2:269:A:H5''   | 61:B2:270:G:H5''   | 1.83                     | 0.58              |
| 9:AO:34:TYR:HB3    | 9:AO:41:PHE:HB2    | 1.86                     | 0.58              |
| 9:AO:40:THR:O      | 9:AO:57:THR:OG1    | 2.22                     | 0.58              |
| 14:AN:127:ARG:HH22 | 61:B2:637:U:H4'    | 1.68                     | 0.58              |
| 28:CN:67:ARG:HH11  | 62:A5:2547:C:H5'   | 1.69                     | 0.58              |
| 28:CN:196:ASN:O    | 78:CL:20:HIS:NE2   | 2.37                     | 0.58              |
| 31:CQ:68:ARG:HD3   | 62:A5:872:A:H61    | 1.69                     | 0.58              |
| 33:CS:86:SER:OG    | 33:CS:87:ARG:N     | 2.36                     | 0.58              |
| 38:CZ:48:ARG:HH21  | 38:CZ:69:LYS:HD2   | 1.68                     | 0.58              |
| 42:Cc:43:ALA:HA    | 42:Cc:97:THR:HA    | 1.86                     | 0.58              |
| 52:Co:80:GLN:NE2   | 62:A5:3323:G:N3    | 2.48                     | 0.58              |
| 61:B2:1966:U:O4    | 61:B2:1985:A:N6    | 2.36                     | 0.58              |
| 62:A5:520:G:N7     | 62:A5:523:C:N4     | 2.52                     | 0.58              |
| 62:A5:937:G:H1'    | 62:A5:967:C:H42    | 1.68                     | 0.58              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 62:A5:1704:A:N6    | 62:A5:1713:U:O4   | 2.36                     | 0.58              |
| 62:A5:3440:C:O2    | 62:A5:3640:A:O2'  | 2.21                     | 0.58              |
| 68:AK:78:ARG:NH1   | 68:AK:84:PRO:O    | 2.37                     | 0.58              |
| 69:AT:50:PRO:O     | 69:AT:53:PHE:CD2  | 2.51                     | 0.58              |
| 70:AF:87:LYS:HD3   | 70:AF:95:ARG:HH12 | 1.69                     | 0.58              |
| 75:AI:4:SER:HA     | 75:AI:29:LEU:HA   | 1.86                     | 0.58              |
| 5:AC:99:THR:OG1    | 5:AC:100:ARG:N    | 2.37                     | 0.58              |
| 9:AO:147:ARG:NH2   | 61:B2:1980:U:OP1  | 2.31                     | 0.58              |
| 19:AY:14:MET:HG2   | 61:B2:865:A:H62   | 1.68                     | 0.58              |
| 33:CS:37:ASN:O     | 33:CS:41:LYS:NZ   | 2.31                     | 0.58              |
| 47:Ck:1:MET:N      | 62:A5:2061:G:O2'  | 2.37                     | 0.58              |
| 47:Ck:28:ASN:O     | 47:Ck:50:LYS:NZ   | 2.36                     | 0.58              |
| 61:B2:992:A:N1     | 61:B2:1085:A:O2'  | 2.37                     | 0.58              |
| 61:B2:1715:G:C3'   | 69:AT:78:ILE:HG21 | 2.34                     | 0.58              |
| 62:A5:313:A:N6     | 62:A5:335:A:N1    | 2.52                     | 0.58              |
| 62:A5:1405:U:OP2   | 77:CO:51:ARG:NE   | 2.37                     | 0.58              |
| 62:A5:2784:C:O2'   | 62:A5:3151:G:N2   | 2.37                     | 0.58              |
| 74:AH:51:GLU:HA    | 74:AH:56:LYS:HA   | 1.84                     | 0.58              |
| 83:Cj:72:ARG:HB3   | 83:Cj:72:ARG:CZ   | 2.34                     | 0.58              |
| 12:AS:130:ARG:NH2  | 12:AS:142:ARG:O   | 2.37                     | 0.58              |
| 18:AV:37:VAL:HG23  | 18:AV:50:SER:HB2  | 1.86                     | 0.58              |
| 19:AY:105:ARG:HD2  | 61:B2:448:C:H3'   | 1.86                     | 0.58              |
| 33:CS:157:ARG:O    | 80:CM:53:ASN:ND2  | 2.37                     | 0.58              |
| 43:Cd:86:ALA:HB3   | 43:Cd:102:TYR:HB3 | 1.86                     | 0.58              |
| 55:CE:208:ALA:HA   | 55:CE:211:LYS:HE3 | 1.86                     | 0.58              |
| 62:A5:1774:C:N4    | 62:A5:1875:G:O6   | 2.35                     | 0.58              |
| 66:Cg:51:LEU:HD21  | 66:Cg:81:CYS:HB3  | 1.86                     | 0.58              |
| 69:AT:20:VAL:HG12  | 69:AT:24:LYS:HE3  | 1.86                     | 0.58              |
| 72:AE:8:HIS:O      | 72:AE:30:ARG:NH1  | 2.37                     | 0.58              |
| 6:CC:294:ARG:NH2   | 39:Cr:73:TYR:OH   | 2.37                     | 0.57              |
| 15:AL:22:LYS:NZ    | 61:B2:211:U:OP1   | 2.37                     | 0.57              |
| 38:CZ:104:VAL:HG23 | 62:A5:1926:A:H4'  | 1.86                     | 0.57              |
| 59:A8:26:U:H2'     | 59:A8:27:C:H6     | 1.69                     | 0.57              |
| 61:B2:1607:U:O2'   | 76:AQ:128:ARG:NH2 | 2.37                     | 0.57              |
| 62:A5:490:G:H22    | 62:A5:510:U:H3    | 1.52                     | 0.57              |
| 62:A5:1069:A:N3    | 62:A5:1091:G:N2   | 2.52                     | 0.57              |
| 62:A5:2202:A:N6    | 62:A5:2769:G:OP1  | 2.37                     | 0.57              |
| 62:A5:2215:G:O2'   | 62:A5:2712:U:O4   | 2.21                     | 0.57              |
| 62:A5:2591:A:N3    | 62:A5:3133:A:O2'  | 2.32                     | 0.57              |
| 62:A5:3838:A:O2'   | 62:A5:3840:G:OP1  | 2.22                     | 0.57              |
| 1:AA:120:ARG:HH22  | 5:AC:250:GLN:HG2  | 1.69                     | 0.57              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 6:CC:119:ASN:OD1   | 62:A5:989:A:O2'    | 2.21                     | 0.57              |
| 10:AX:119:ARG:NH2  | 61:B2:1223:U:OP2   | 2.36                     | 0.57              |
| 10:AX:123:VAL:HG13 | 10:AX:124:LYS:HG2  | 1.85                     | 0.57              |
| 14:AN:23:PRO:HB2   | 14:AN:26:LEU:HB2   | 1.85                     | 0.57              |
| 28:CN:85:LYS:NZ    | 62:A5:48:U:OP2     | 2.37                     | 0.57              |
| 37:CY:88:GLU:HG3   | 37:CY:94:ASN:HB3   | 1.86                     | 0.57              |
| 55:CE:138:ARG:NH1  | 62:A5:3841:C:O2    | 2.37                     | 0.57              |
| 61:B2:193:U:H5''   | 61:B2:919:A:H61    | 1.69                     | 0.57              |
| 61:B2:275:U:H3     | 61:B2:290:A:H2     | 1.52                     | 0.57              |
| 62:A5:99:A:C5      | 62:A5:100:G:H1'    | 2.39                     | 0.57              |
| 62:A5:1781:U:O3'   | 62:A5:1797:A:N6    | 2.37                     | 0.57              |
| 62:A5:2599:G:N2    | 62:A5:2602:A:OP2   | 2.34                     | 0.57              |
| 62:A5:3208:A:OP1   | 62:A5:3211:A:N6    | 2.36                     | 0.57              |
| 62:A5:3448:U:O2    | 62:A5:3467:A:N6    | 2.37                     | 0.57              |
| 64:AW:36:LYS:HB3   | 64:AW:110:ILE:HG21 | 1.86                     | 0.57              |
| 4:CB:384:ASP:OD2   | 65:CW:12:LYS:NZ    | 2.36                     | 0.57              |
| 5:AC:254:ASP:OD1   | 5:AC:254:ASP:N     | 2.37                     | 0.57              |
| 26:AJ:73:PHE:HA    | 72:AE:252:ARG:HH22 | 1.67                     | 0.57              |
| 30:CD:152:ARG:HE   | 62:A5:3195:G:H5'   | 1.68                     | 0.57              |
| 41:Cb:2:ALA:N      | 62:A5:3149:U:OP2   | 2.38                     | 0.57              |
| 55:CE:42:ARG:HH12  | 62:A5:699:U:H1'    | 1.68                     | 0.57              |
| 59:A8:42:A:H61     | 59:A8:98:U:H3      | 1.52                     | 0.57              |
| 61:B2:138:U:O2'    | 61:B2:271:A:N3     | 2.36                     | 0.57              |
| 61:B2:1244:C:N4    | 61:B2:1814:G:O6    | 2.36                     | 0.57              |
| 62:A5:1205:U:N3    | 62:A5:1206:G:O6    | 2.37                     | 0.57              |
| 62:A5:1979:A:H1'   | 66:Cg:21:ARG:HH22  | 1.69                     | 0.57              |
| 62:A5:2503:G:H1    | 62:A5:2707:C:H42   | 1.51                     | 0.57              |
| 62:A5:2929:U:H3    | 62:A5:2989:G:H1    | 1.51                     | 0.57              |
| 62:A5:3926:C:H5''  | 75:AI:170:SER:HA   | 1.86                     | 0.57              |
| 69:AT:6:VAL:HG11   | 69:AT:136:ASN:CG   | 2.29                     | 0.57              |
| 69:AT:59:SER:CB    | 69:AT:63:HIS:HD2   | 2.18                     | 0.57              |
| 2:CA:3:ARG:NH1     | 62:A5:1109:G:N7    | 2.52                     | 0.57              |
| 4:CB:117:ARG:HD2   | 4:CB:177:LYS:HE2   | 1.85                     | 0.57              |
| 5:AC:43:TRP:HB3    | 5:AC:54:ARG:HH21   | 1.68                     | 0.57              |
| 5:AC:106:ARG:NH2   | 61:B2:1378:C:OP1   | 2.37                     | 0.57              |
| 12:AS:39:ARG:HG3   | 69:AT:38:LYS:CE    | 2.34                     | 0.57              |
| 17:AP:84:ARG:HG3   | 61:B2:1749:C:H42   | 1.70                     | 0.57              |
| 28:CN:202:ARG:NH1  | 62:A5:842:A:OP1    | 2.37                     | 0.57              |
| 53:CJ:113:GLY:HA3  | 62:A5:3206:A:H5''  | 1.84                     | 0.57              |
| 54:CH:12:ILE:HG23  | 54:CH:16:ILE:HD11  | 1.86                     | 0.57              |
| 59:A8:108:A:C6     | 83:Cj:29:LEU:HD11  | 2.39                     | 0.57              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 61:B2:466:G:H2'    | 61:B2:467:G:H8     | 1.70                     | 0.57              |
| 62:A5:1389:C:H42   | 62:A5:1525:G:H22   | 1.52                     | 0.57              |
| 62:A5:3800:G:H22   | 62:A5:3809:U:H3    | 1.50                     | 0.57              |
| 69:AT:55:VAL:O     | 69:AT:55:VAL:HG12  | 2.02                     | 0.57              |
| 12:AS:38:ARG:HB3   | 69:AT:45:LEU:HD21  | 1.85                     | 0.57              |
| 17:AP:13:ARG:HH22  | 17:AP:25:LEU:HD23  | 1.69                     | 0.57              |
| 25:Af:138:ARG:HG3  | 25:Af:149:VAL:HG13 | 1.87                     | 0.57              |
| 39:Cr:118:ALA:HA   | 39:Cr:121:VAL:HG12 | 1.87                     | 0.57              |
| 62:A5:3468:G:H2'   | 62:A5:3469:G:H8    | 1.70                     | 0.57              |
| 69:AT:10:ASP:CG    | 76:AQ:44:ILE:HA    | 2.28                     | 0.57              |
| 73:AG:1:MET:N      | 73:AG:18:VAL:O     | 2.37                     | 0.57              |
| 75:AI:81:VAL:HG23  | 75:AI:102:VAL:HG12 | 1.85                     | 0.57              |
| 77:CO:108:ASP:OD1  | 77:CO:108:ASP:N    | 2.37                     | 0.57              |
| 4:CB:371:SER:OG    | 4:CB:372:SER:N     | 2.38                     | 0.57              |
| 13:Ad:21:CYS:H     | 13:Ad:30:LEU:HD22  | 1.70                     | 0.57              |
| 31:CQ:11:ARG:NH2   | 62:A5:1173:U:OP2   | 2.36                     | 0.57              |
| 31:CQ:156:PRO:HB3  | 31:CQ:188:LYS:HE2  | 1.86                     | 0.57              |
| 34:CT:108:ARG:O    | 34:CT:112:ASN:ND2  | 2.38                     | 0.57              |
| 38:CZ:93:GLU:OE2   | 38:CZ:116:LYS:NZ   | 2.36                     | 0.57              |
| 39:Cr:62:LYS:HB3   | 39:Cr:125:GLN:HB3  | 1.86                     | 0.57              |
| 50:Cn:2:ARG:NH2    | 61:B2:1979:C:OP2   | 2.38                     | 0.57              |
| 61:B2:625:U:O4     | 61:B2:1174:A:N6    | 2.37                     | 0.57              |
| 62:A5:1680:U:H2'   | 62:A5:1681:G:H8    | 1.70                     | 0.57              |
| 83:Cj:20:ARG:HG2   | 83:Cj:20:ARG:HH11  | 1.70                     | 0.57              |
| 5:AC:100:ARG:NH2   | 61:B2:1234:G:O2'   | 2.37                     | 0.57              |
| 6:CC:329:ILE:HD13  | 6:CC:336:GLU:HB2   | 1.87                     | 0.57              |
| 9:AO:57:THR:OG1    | 9:AO:58:GLY:N      | 2.38                     | 0.57              |
| 9:AO:98:ARG:NH1    | 61:B2:1005:G:OP2   | 2.38                     | 0.57              |
| 26:AJ:145:ILE:HG22 | 26:AJ:147:SER:H    | 1.69                     | 0.57              |
| 30:CD:158:ARG:NH1  | 58:A7:47:C:OP2     | 2.38                     | 0.57              |
| 52:Co:77:TYR:HH    | 62:A5:3302:G:HO2'  | 1.52                     | 0.57              |
| 61:B2:1771:U:OP1   | 76:AQ:148:ARG:NH1  | 2.31                     | 0.57              |
| 62:A5:1349:A:H2'   | 62:A5:1350:A:H8    | 1.69                     | 0.57              |
| 62:A5:1596:A:H8    | 62:A5:1598:A:C6    | 2.22                     | 0.57              |
| 62:A5:1624:G:N2    | 62:A5:1665:C:O2    | 2.31                     | 0.57              |
| 25:Af:87:THR:HA    | 61:B2:1637:G:H22   | 1.70                     | 0.57              |
| 28:CN:19:MET:O     | 28:CN:23:LEU:N     | 2.34                     | 0.57              |
| 53:CJ:113:GLY:HA2  | 53:CJ:134:ASP:HA   | 1.87                     | 0.57              |
| 61:B2:1697:A:P     | 69:AT:41:LYS:HE3   | 2.43                     | 0.57              |
| 62:A5:62:G:O2'     | 62:A5:64:A:O2'     | 2.15                     | 0.57              |
| 62:A5:677:G:O6     | 62:A5:743:C:N4     | 2.38                     | 0.57              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 62:A5:850:A:OP1    | 78:CL:65:TYR:OH    | 2.22                     | 0.57              |
| 62:A5:1426:U:H2'   | 62:A5:1427:G:H8    | 1.69                     | 0.57              |
| 3:AB:28:LYS:NZ     | 3:AB:50:ASN:OD1    | 2.38                     | 0.57              |
| 3:AB:206:ARG:HH21  | 61:B2:1145:U:H5'   | 1.70                     | 0.57              |
| 3:AB:228:VAL:HA    | 3:AB:231:LEU:HB3   | 1.86                     | 0.57              |
| 8:AU:34:LEU:HB3    | 8:AU:89:ARG:HH12   | 1.68                     | 0.57              |
| 30:CD:47:PRO:HG3   | 30:CD:68:ARG:HH21  | 1.67                     | 0.57              |
| 30:CD:143:ARG:HA   | 30:CD:172:ASN:HB2  | 1.85                     | 0.57              |
| 32:CR:16:ARG:NH2   | 62:A5:2068:A:OP1   | 2.35                     | 0.57              |
| 61:B2:16:G:H21     | 61:B2:1226:A:H62   | 1.53                     | 0.57              |
| 61:B2:145:A:N7     | 61:B2:163:C:N4     | 2.47                     | 0.57              |
| 61:B2:1549:U:H3    | 61:B2:1561:G:H22   | 1.53                     | 0.57              |
| 62:A5:1513:C:H2'   | 62:A5:1514:U:H6    | 1.68                     | 0.57              |
| 62:A5:1654:C:H2'   | 62:A5:1655:A:H8    | 1.68                     | 0.57              |
| 77:CO:132:ARG:NH2  | 77:CO:133:SER:O    | 2.38                     | 0.57              |
| 4:CB:284:ILE:HA    | 4:CB:333:ILE:HG22  | 1.85                     | 0.57              |
| 4:CB:391:PRO:O     | 62:A5:3943:G:N2    | 2.37                     | 0.57              |
| 16:AR:25:THR:O     | 16:AR:31:ASN:ND2   | 2.37                     | 0.57              |
| 32:CR:67:THR:O     | 32:CR:71:ARG:NH1   | 2.38                     | 0.57              |
| 61:B2:1310:A:H1'   | 61:B2:1348:A:H61   | 1.70                     | 0.57              |
| 62:A5:1275:A:O2'   | 62:A5:1311:U:OP1   | 2.23                     | 0.57              |
| 62:A5:1521:G:N2    | 62:A5:1522:G:N7    | 2.50                     | 0.57              |
| 62:A5:2721:C:N4    | 62:A5:2722:U:O4    | 2.38                     | 0.57              |
| 70:AF:163:VAL:HG23 | 70:AF:228:ARG:HE   | 1.69                     | 0.57              |
| 7:Ag:5:LEU:HD23    | 7:Ag:311:TRP:HB3   | 1.87                     | 0.56              |
| 31:CQ:54:SER:OG    | 31:CQ:56:ILE:O     | 2.21                     | 0.56              |
| 34:CT:69:GLN:NE2   | 62:A5:3270:G:OP1   | 2.37                     | 0.56              |
| 45:Cf:1:MET:HE1    | 62:A5:642:A:H61    | 1.68                     | 0.56              |
| 56:CG:63:PRO:HB3   | 62:A5:1801:U:H2'   | 1.87                     | 0.56              |
| 62:A5:796:A:H61    | 62:A5:2749:G:H21   | 1.52                     | 0.56              |
| 62:A5:1979:A:O2'   | 66:Cg:21:ARG:NH1   | 2.37                     | 0.56              |
| 6:CC:347:GLU:O     | 6:CC:350:THR:OG1   | 2.22                     | 0.56              |
| 11:AM:108:ARG:HB3  | 11:AM:110:VAL:HG13 | 1.87                     | 0.56              |
| 48:Cl:48:LYS:NZ    | 62:A5:1736:G:OP1   | 2.35                     | 0.56              |
| 58:A7:79:U:O2      | 58:A7:98:G:N1      | 2.37                     | 0.56              |
| 60:Cz:27:GLY:HA3   | 62:A5:2863:U:H5'   | 1.87                     | 0.56              |
| 61:B2:45:U:H2'     | 61:B2:46:A:H2'     | 1.86                     | 0.56              |
| 61:B2:1882:C:N4    | 61:B2:1900:U:OP2   | 2.38                     | 0.56              |
| 62:A5:1751:U:O5'   | 62:A5:2732:C:O2'   | 2.23                     | 0.56              |
| 62:A5:1950:A:OP1   | 66:Cg:74:ARG:NH2   | 2.35                     | 0.56              |
| 1:AA:85:ARG:NH2    | 1:AA:201:LEU:O     | 2.38                     | 0.56              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:CA:133:TYR:HB3   | 2:CA:168:ILE:HG13  | 1.86                     | 0.56              |
| 14:AN:124:ARG:NE   | 61:B2:1053:A:OP2   | 2.38                     | 0.56              |
| 16:AR:36:GLU:OE2   | 16:AR:47:ARG:NH2   | 2.38                     | 0.56              |
| 21:Aa:15:ARG:NH2   | 61:B2:1023:G:N7    | 2.53                     | 0.56              |
| 21:Aa:88:SER:OG    | 21:Aa:89:ARG:N     | 2.38                     | 0.56              |
| 22:Ab:65:GLN:HG3   | 22:Ab:73:LEU:HG    | 1.86                     | 0.56              |
| 28:CN:30:TYR:O     | 28:CN:31:ARG:NH1   | 2.33                     | 0.56              |
| 30:CD:62:VAL:HB    | 30:CD:78:ALA:HB3   | 1.87                     | 0.56              |
| 33:CS:55:LYS:O     | 33:CS:58:THR:N     | 2.36                     | 0.56              |
| 39:Cr:91:ARG:HE    | 39:Cr:92:ARG:HG2   | 1.69                     | 0.56              |
| 43:Cd:14:ILE:N     | 43:Cd:16:GLU:OE1   | 2.38                     | 0.56              |
| 44:Ce:102:VAL:O    | 44:Ce:107:ARG:NH2  | 2.34                     | 0.56              |
| 46:Ci:68:MET:HA    | 46:Ci:100:LEU:HD21 | 1.87                     | 0.56              |
| 61:B2:96:C:O2      | 61:B2:430:A:O2'    | 2.23                     | 0.56              |
| 61:B2:871:G:O6     | 72:AE:51:ARG:NH1   | 2.38                     | 0.56              |
| 61:B2:1142:U:H3    | 61:B2:1151:G:H1    | 1.51                     | 0.56              |
| 61:B2:1715:G:O5'   | 69:AT:78:ILE:HD12  | 1.98                     | 0.56              |
| 61:B2:1984:G:H2'   | 61:B2:1985:A:H8    | 1.70                     | 0.56              |
| 62:A5:310:A:OP1    | 62:A5:2810:A:O2'   | 2.23                     | 0.56              |
| 62:A5:489:U:H3     | 62:A5:511:G:H1     | 1.51                     | 0.56              |
| 62:A5:944:G:H5'    | 62:A5:959:U:H3     | 1.68                     | 0.56              |
| 62:A5:1951:C:H5''  | 66:Cg:72:VAL:HG11  | 1.87                     | 0.56              |
| 67:CU:195:ILE:HG23 | 67:CU:245:HIS:HB2  | 1.88                     | 0.56              |
| 68:AK:31:LYS:O     | 68:AK:40:ASN:ND2   | 2.39                     | 0.56              |
| 69:AT:48:TYR:O     | 69:AT:49:ASP:OD1   | 2.23                     | 0.56              |
| 69:AT:127:GLY:HA2  | 69:AT:131:LEU:HB2  | 1.87                     | 0.56              |
| 75:AI:152:LEU:O    | 75:AI:156:LYS:NZ   | 2.35                     | 0.56              |
| 78:CL:103:ASN:ND2  | 78:CL:108:SER:OG   | 2.32                     | 0.56              |
| 11:AM:25:LEU:HB2   | 11:AM:85:ARG:HH22  | 1.71                     | 0.56              |
| 11:AM:61:GLU:HB3   | 11:AM:86:VAL:HB    | 1.88                     | 0.56              |
| 12:AS:39:ARG:NH1   | 61:B2:1757:G:OP2   | 2.39                     | 0.56              |
| 33:CS:156:GLN:OE1  | 80:CM:53:ASN:ND2   | 2.30                     | 0.56              |
| 45:Cf:44:TYR:HA    | 55:CE:237:TYR:HE1  | 1.70                     | 0.56              |
| 61:B2:386:C:OP2    | 72:AE:10:LYS:NZ    | 2.35                     | 0.56              |
| 61:B2:401:G:N1     | 61:B2:404:A:OP2    | 2.38                     | 0.56              |
| 62:A5:1462:U:N3    | 62:A5:1484:U:O4    | 2.38                     | 0.56              |
| 62:A5:2910:C:H42   | 62:A5:3123:G:H1    | 1.53                     | 0.56              |
| 63:Ac:40:ARG:NH1   | 63:Ac:56:GLU:O     | 2.37                     | 0.56              |
| 64:AW:9:ASP:OD1    | 64:AW:9:ASP:N      | 2.36                     | 0.56              |
| 81:B:17:G:OP2      | 81:B:59:A:O2'      | 2.24                     | 0.56              |
| 1:AA:128:ASN:O     | 1:AA:131:HIS:ND1   | 2.32                     | 0.56              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:AB:67:PHE:HD2    | 3:AB:89:LEU:HD12   | 1.70                     | 0.56              |
| 6:CC:3:LEU:HB3     | 6:CC:6:ALA:HB2     | 1.87                     | 0.56              |
| 31:CQ:158:VAL:O    | 31:CQ:161:SER:OG   | 2.24                     | 0.56              |
| 37:CY:45:ARG:NH2   | 62:A5:247:C:OP2    | 2.39                     | 0.56              |
| 59:A8:109:U:O4     | 59:A8:111:G:N2     | 2.38                     | 0.56              |
| 62:A5:1341:G:N2    | 62:A5:1344:A:OP2   | 2.38                     | 0.56              |
| 62:A5:2214:G:O6    | 62:A5:2715:C:N4    | 2.38                     | 0.56              |
| 62:A5:3221:A:N6    | 62:A5:3234:A:O2'   | 2.39                     | 0.56              |
| 69:AT:29:LYS:HZ2   | 69:AT:106:ALA:C    | 2.13                     | 0.56              |
| 69:AT:60:ILE:HG22  | 69:AT:60:ILE:O     | 2.04                     | 0.56              |
| 2:CA:117:GLU:OE2   | 2:CA:124:GLY:N     | 2.39                     | 0.56              |
| 8:AU:57:ARG:NH2    | 61:B2:1576:A:OP1   | 2.38                     | 0.56              |
| 12:AS:83:PHE:CZ    | 69:AT:36:ILE:HG22  | 2.38                     | 0.56              |
| 27:Ca:9:THR:HG22   | 27:Ca:12:LEU:HD12  | 1.87                     | 0.56              |
| 30:CD:118:LEU:HD21 | 30:CD:135:VAL:HG21 | 1.87                     | 0.56              |
| 30:CD:212:GLU:HA   | 30:CD:219:PHE:HZ   | 1.71                     | 0.56              |
| 31:CQ:64:GLN:O     | 62:A5:872:A:N6     | 2.39                     | 0.56              |
| 33:CS:65:LYS:NZ    | 62:A5:565:C:O2'    | 2.38                     | 0.56              |
| 36:CX:220:LEU:HD11 | 36:CX:254:GLN:HB3  | 1.88                     | 0.56              |
| 47:Ck:59:SER:O     | 47:Ck:59:SER:OG    | 2.23                     | 0.56              |
| 55:CE:59:LYS:O     | 55:CE:63:LYS:NZ    | 2.39                     | 0.56              |
| 59:A8:17:U:HO2'    | 62:A5:1636:G:HO2'  | 1.54                     | 0.56              |
| 61:B2:1066:A:N3    | 61:B2:1970:U:O2'   | 2.37                     | 0.56              |
| 61:B2:1199:G:N2    | 61:B2:1223:U:O2    | 2.39                     | 0.56              |
| 62:A5:1967:G:N2    | 62:A5:2114:U:O4    | 2.38                     | 0.56              |
| 62:A5:2853:A:N6    | 62:A5:2863:U:O4    | 2.39                     | 0.56              |
| 69:AT:23:LYS:CA    | 69:AT:28:LEU:HD21  | 2.36                     | 0.56              |
| 74:AH:64:ILE:HG22  | 74:AH:67:GLN:HB3   | 1.87                     | 0.56              |
| 3:AB:107:ASP:HA    | 3:AB:217:LYS:HA    | 1.86                     | 0.56              |
| 9:AO:142:ARG:HH22  | 21:Aa:24:THR:HA    | 1.70                     | 0.56              |
| 51:Cp:84:ARG:HG2   | 51:Cp:87:ARG:HH12  | 1.70                     | 0.56              |
| 54:CH:58:TRP:HD1   | 62:A5:3728:A:H1'   | 1.70                     | 0.56              |
| 61:B2:507:C:O2     | 61:B2:509:C:N4     | 2.39                     | 0.56              |
| 61:B2:546:A:O2'    | 61:B2:548:G:N2     | 2.39                     | 0.56              |
| 61:B2:1715:G:H5'   | 69:AT:78:ILE:HD12  | 1.82                     | 0.56              |
| 62:A5:535:A:OP2    | 62:A5:538:A:N6     | 2.39                     | 0.56              |
| 62:A5:595:U:H3     | 62:A5:614:G:H1     | 1.53                     | 0.56              |
| 62:A5:1168:G:N7    | 62:A5:1169:C:N4    | 2.53                     | 0.56              |
| 62:A5:1382:U:N3    | 62:A5:1547:A:N1    | 2.53                     | 0.56              |
| 62:A5:2216:A:H4'   | 62:A5:2217:A:H5'   | 1.86                     | 0.56              |
| 62:A5:3894:C:H42   | 62:A5:3961:G:H1    | 1.54                     | 0.56              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 6:CC:134:SER:OG   | 6:CC:135:GLY:N     | 2.38                     | 0.56              |
| 10:AX:1:MET:SD    | 61:B2:630:A:N6     | 2.78                     | 0.56              |
| 16:AR:49:LYS:HD3  | 61:B2:1583:A:H61   | 1.71                     | 0.56              |
| 17:AP:32:PRO:HG2  | 17:AP:36:LEU:HD23  | 1.88                     | 0.56              |
| 26:AJ:89:ASP:H    | 26:AJ:92:ARG:HH21  | 1.52                     | 0.56              |
| 43:CD:24:ILE:HD11 | 43:CD:26:LEU:HD13  | 1.87                     | 0.56              |
| 61:B2:1757:G:OP1  | 69:AT:38:LYS:CE    | 2.54                     | 0.56              |
| 61:B2:1847:A:N3   | 62:A5:2680:G:O2'   | 2.30                     | 0.56              |
| 62:A5:1013:G:N1   | 62:A5:1014:U:O2    | 2.39                     | 0.56              |
| 62:A5:1215:A:H2'  | 62:A5:1216:A:H8    | 1.71                     | 0.56              |
| 62:A5:1955:A:OP2  | 66:Cg:68:ARG:NE    | 2.39                     | 0.56              |
| 66:Cg:67:LYS:HA   | 66:Cg:70:LYS:HD2   | 1.88                     | 0.56              |
| 71:CF:97:ARG:NH1  | 71:CF:118:ARG:O    | 2.39                     | 0.56              |
| 4:CB:70:LYS:NZ    | 4:CB:71:GLU:O      | 2.39                     | 0.56              |
| 4:CB:77:THR:HG21  | 4:CB:337:CYS:H     | 1.70                     | 0.56              |
| 7:Ag:193:ASN:HB2  | 7:Ag:216:LYS:HE2   | 1.87                     | 0.56              |
| 10:AX:26:ASP:OD1  | 10:AX:26:ASP:N     | 2.39                     | 0.56              |
| 29:CI:61:SER:OG   | 29:CI:63:GLU:OE1   | 2.24                     | 0.56              |
| 35:CP:108:ASP:N   | 35:CP:108:ASP:OD1  | 2.38                     | 0.56              |
| 61:B2:951:A:OP1   | 64:AW:28:ARG:NH1   | 2.39                     | 0.56              |
| 61:B2:1956:U:OP2  | 82:v:29:G:O2'      | 2.23                     | 0.56              |
| 62:A5:360:A:O4'   | 62:A5:362:A:N6     | 2.39                     | 0.56              |
| 62:A5:1724:A:N3   | 66:Cg:4:ARG:NH1    | 2.54                     | 0.56              |
| 62:A5:2933:A:N1   | 62:A5:2985:U:N3    | 2.48                     | 0.56              |
| 62:A5:3254:U:H2'  | 62:A5:3255:G:H8    | 1.70                     | 0.56              |
| 69:AT:29:LYS:NZ   | 69:AT:106:ALA:CA   | 2.66                     | 0.56              |
| 74:AH:46:ARG:NH1  | 74:AH:47:ALA:O     | 2.39                     | 0.56              |
| 12:AS:15:ILE:HD11 | 12:AS:33:ILE:HG12  | 1.88                     | 0.56              |
| 62:A5:1557:U:O2   | 62:A5:1604:G:N2    | 2.39                     | 0.56              |
| 69:AT:68:SER:HB2  | 69:AT:69:PRO:CD    | 2.36                     | 0.56              |
| 80:CM:148:ARG:HA  | 80:CM:151:LEU:HD13 | 1.88                     | 0.56              |
| 7:Ag:79:ALA:HB3   | 7:Ag:91:TRP:HB2    | 1.88                     | 0.55              |
| 14:AN:75:MET:O    | 14:AN:80:LEU:N     | 2.37                     | 0.55              |
| 40:Ch:46:LYS:NZ   | 59:A8:78:G:O2'     | 2.38                     | 0.55              |
| 42:Cc:53:PRO:O    | 42:Cc:57:LYS:N     | 2.38                     | 0.55              |
| 43:CD:22:CYS:O    | 43:CD:82:ARG:NH1   | 2.39                     | 0.55              |
| 45:Cf:94:TYR:HB2  | 45:Cf:148:ILE:HB   | 1.89                     | 0.55              |
| 47:Ck:17:ARG:NH2  | 62:A5:2140:C:O3'   | 2.40                     | 0.55              |
| 61:B2:964:G:OP2   | 61:B2:1023:G:N2    | 2.37                     | 0.55              |
| 61:B2:1445:A:C1'  | 69:AT:133:ARG:NH2  | 2.68                     | 0.55              |
| 62:A5:3:A:O2'     | 62:A5:3116:A:OP2   | 2.24                     | 0.55              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 62:A5:795:A:N6    | 62:A5:799:A:N3     | 2.53                     | 0.55              |
| 62:A5:1702:G:H2'  | 62:A5:1703:A:H8    | 1.70                     | 0.55              |
| 62:A5:2509:G:H2'  | 62:A5:2510:A:H4'   | 1.88                     | 0.55              |
| 62:A5:3754:C:OP1  | 80:CM:56:HIS:ND1   | 2.38                     | 0.55              |
| 6:CC:66:SER:O     | 6:CC:66:SER:OG     | 2.20                     | 0.55              |
| 9:AO:66:ARG:HG3   | 61:B2:992:A:H5''   | 1.87                     | 0.55              |
| 30:CD:52:ILE:HD13 | 58:A7:6:C:H4'      | 1.88                     | 0.55              |
| 31:CQ:146:ARG:HA  | 62:A5:986:A:H3'    | 1.86                     | 0.55              |
| 34:CT:148:ILE:HA  | 34:CT:150:LEU:HD12 | 1.87                     | 0.55              |
| 38:CZ:67:LYS:NZ   | 62:A5:1941:A:OP1   | 2.38                     | 0.55              |
| 61:B2:1401:U:O2'  | 61:B2:1415:G:N2    | 2.38                     | 0.55              |
| 75:AI:20:SER:OG   | 75:AI:21:LEU:N     | 2.33                     | 0.55              |
| 4:CB:228:PHE:O    | 62:A5:2202:A:O2'   | 2.24                     | 0.55              |
| 6:CC:389:LYS:NZ   | 62:A5:697:U:O2     | 2.37                     | 0.55              |
| 12:AS:76:GLN:O    | 12:AS:78:LYS:NZ    | 2.39                     | 0.55              |
| 27:Ca:39:MET:O    | 27:Ca:43:ARG:NH2   | 2.39                     | 0.55              |
| 33:CS:24:GLN:HG2  | 34:CT:144:LEU:HD11 | 1.88                     | 0.55              |
| 33:CS:118:ARG:NH1 | 62:A5:1510:G:O3'   | 2.39                     | 0.55              |
| 37:CY:31:SER:HA   | 37:CY:48:PRO:HA    | 1.86                     | 0.55              |
| 45:Cf:46:ARG:HE   | 45:Cf:49:ARG:HH21  | 1.54                     | 0.55              |
| 55:CE:33:TYR:O    | 55:CE:37:GLN:NE2   | 2.39                     | 0.55              |
| 61:B2:553:A:N6    | 61:B2:602:A:O5'    | 2.39                     | 0.55              |
| 61:B2:624:G:H22   | 61:B2:1194:C:H1'   | 1.70                     | 0.55              |
| 61:B2:1551:C:N4   | 61:B2:1559:A:OP2   | 2.38                     | 0.55              |
| 61:B2:1727:U:C5   | 70:AF:190:ILE:HG13 | 2.41                     | 0.55              |
| 62:A5:344:U:OP2   | 78:CL:33:ARG:NH2   | 2.33                     | 0.55              |
| 62:A5:1237:G:H8   | 62:A5:1240:A:H8    | 1.54                     | 0.55              |
| 62:A5:1725:A:H5'' | 62:A5:2182:G:H21   | 1.72                     | 0.55              |
| 64:AW:80:ASP:OD1  | 64:AW:80:ASP:N     | 2.38                     | 0.55              |
| 69:AT:11:GLN:O    | 69:AT:15:THR:HG23  | 2.06                     | 0.55              |
| 69:AT:23:LYS:HB3  | 69:AT:28:LEU:HD21  | 1.86                     | 0.55              |
| 69:AT:50:PRO:C    | 69:AT:53:PHE:HD2   | 2.14                     | 0.55              |
| 3:AB:46:LYS:H     | 9:AO:27:VAL:HG23   | 1.72                     | 0.55              |
| 5:AC:191:PRO:HD3  | 26:AJ:19:ARG:HH12  | 1.70                     | 0.55              |
| 7:Ag:8:ARG:HB2    | 7:Ag:310:VAL:HG23  | 1.87                     | 0.55              |
| 12:AS:141:ARG:HG3 | 12:AS:142:ARG:HG3  | 1.87                     | 0.55              |
| 36:CX:177:ARG:NH2 | 57:A9:9:C:O2'      | 2.39                     | 0.55              |
| 47:Ck:53:ALA:O    | 47:Ck:57:LYS:N     | 2.37                     | 0.55              |
| 61:B2:257:U:O2    | 72:AE:130:GLN:NE2  | 2.38                     | 0.55              |
| 61:B2:397:G:OP1   | 75:AI:24:LYS:NZ    | 2.39                     | 0.55              |
| 61:B2:1424:A:N1   | 61:B2:1603:G:N2    | 2.41                     | 0.55              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 62:A5:1149:C:O2'   | 62:A5:1171:G:OP1   | 2.25                     | 0.55              |
| 62:A5:1767:A:O2'   | 62:A5:1769:U:OP2   | 2.21                     | 0.55              |
| 70:AF:54:VAL:HG13  | 70:AF:60:GLN:HG3   | 1.88                     | 0.55              |
| 4:CB:223:THR:OG1   | 62:A5:3583:C:OP1   | 2.22                     | 0.55              |
| 10:AX:17:ARG:HD2   | 10:AX:21:ARG:HH21  | 1.70                     | 0.55              |
| 12:AS:120:HIS:HB2  | 17:AP:121:GLU:HA   | 1.88                     | 0.55              |
| 19:AY:78:ASP:OD1   | 19:AY:78:ASP:N     | 2.40                     | 0.55              |
| 23:AD:11:ARG:NH2   | 61:B2:1681:U:OP1   | 2.40                     | 0.55              |
| 29:CI:4:ARG:HH11   | 29:CI:99:ILE:HG23  | 1.70                     | 0.55              |
| 29:CI:56:GLU:HB2   | 29:CI:58:GLU:HB2   | 1.87                     | 0.55              |
| 35:CP:111:ARG:HH21 | 35:CP:153:LYS:HB2  | 1.71                     | 0.55              |
| 36:CX:159:ARG:NH1  | 57:A9:24:G:O5'     | 2.40                     | 0.55              |
| 45:Cf:152:LEU:HD12 | 55:CE:104:LEU:HD11 | 1.88                     | 0.55              |
| 55:CE:236:GLN:NE2  | 80:CM:106:ASP:OD1  | 2.40                     | 0.55              |
| 61:B2:1319:A:N3    | 61:B2:1341:C:N4    | 2.54                     | 0.55              |
| 61:B2:1426:A:H61   | 61:B2:1578:U:H3    | 1.55                     | 0.55              |
| 62:A5:1991:A:OP1   | 67:CU:273:ARG:NE   | 2.34                     | 0.55              |
| 64:AW:25:VAL:HB    | 64:AW:63:VAL:HB    | 1.87                     | 0.55              |
| 72:AE:45:LEU:HD21  | 72:AE:80:PRO:HB2   | 1.87                     | 0.55              |
| 77:CO:201:TYR:OH   | 80:CM:113:ARG:NH2  | 2.40                     | 0.55              |
| 5:AC:218:ASN:ND2   | 61:B2:1385:U:O2    | 2.39                     | 0.55              |
| 12:AS:31:THR:HG21  | 12:AS:38:ARG:HG3   | 1.87                     | 0.55              |
| 31:CQ:65:ARG:NH2   | 62:A5:911:A:OP1    | 2.39                     | 0.55              |
| 32:CR:64:ARG:NH1   | 62:A5:2001:U:OP1   | 2.39                     | 0.55              |
| 36:CX:162:ARG:NH1  | 62:A5:1861:A:OP1   | 2.39                     | 0.55              |
| 45:Cf:124:ILE:HA   | 45:Cf:131:VAL:HG22 | 1.89                     | 0.55              |
| 45:Cf:154:PRO:HB3  | 55:CE:143:ARG:HB3  | 1.88                     | 0.55              |
| 61:B2:1782:G:H4'   | 69:AT:92:PHE:CZ    | 2.41                     | 0.55              |
| 62:A5:1725:A:OP2   | 62:A5:2182:G:N2    | 2.39                     | 0.55              |
| 77:CO:12:ASP:HB2   | 77:CO:119:ARG:HD3  | 1.89                     | 0.55              |
| 14:AN:124:ARG:NH1  | 61:B2:636:G:OP1    | 2.38                     | 0.55              |
| 29:CI:87:ILE:HG23  | 29:CI:136:MET:HE1  | 1.89                     | 0.55              |
| 36:CX:189:ARG:HH22 | 36:CX:191:ARG:HE   | 1.55                     | 0.55              |
| 47:Ck:3:ARG:NH1    | 62:A5:2011:A:O2'   | 2.40                     | 0.55              |
| 54:CH:175:ASP:N    | 54:CH:175:ASP:OD1  | 2.37                     | 0.55              |
| 61:B2:1121:C:HO2'  | 64:AW:2:VAL:N      | 2.03                     | 0.55              |
| 61:B2:1314:G:O5'   | 61:B2:1343:A:N6    | 2.40                     | 0.55              |
| 62:A5:676:A:H2     | 62:A5:746:G:H22    | 1.55                     | 0.55              |
| 62:A5:1696:A:H5''  | 62:A5:1697:U:H5'   | 1.88                     | 0.55              |
| 74:AH:94:ALA:O     | 74:AH:96:ARG:NH1   | 2.38                     | 0.55              |
| 3:AB:167:ILE:HD11  | 3:AB:207:ILE:HB    | 1.89                     | 0.55              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 3:AB:193:LEU:O    | 3:AB:198:LYS:NZ    | 2.39                     | 0.55              |
| 4:CB:232:THR:HG21 | 4:CB:249:ARG:HG2   | 1.88                     | 0.55              |
| 4:CB:374:MET:O    | 62:A5:3904:G:O2'   | 2.25                     | 0.55              |
| 6:CC:296:LEU:O    | 62:A5:1564:G:O2'   | 2.23                     | 0.55              |
| 29:CI:140:SER:OG  | 29:CI:141:SER:N    | 2.39                     | 0.55              |
| 31:CQ:68:ARG:NH1  | 62:A5:872:A:N1     | 2.54                     | 0.55              |
| 42:Cc:35:LEU:HD23 | 42:Cc:38:LEU:HD23  | 1.88                     | 0.55              |
| 45:Cf:65:ASN:O    | 45:Cf:66:GLN:NE2   | 2.40                     | 0.55              |
| 45:Cf:120:LYS:NZ  | 62:A5:659:U:OP1    | 2.37                     | 0.55              |
| 47:Ck:9:LYS:O     | 47:Ck:9:LYS:NZ     | 2.37                     | 0.55              |
| 48:Cl:16:LYS:O    | 48:Cl:42:ARG:NH1   | 2.40                     | 0.55              |
| 55:CE:36:ALA:HA   | 55:CE:39:TYR:HB3   | 1.88                     | 0.55              |
| 61:B2:1670:G:O2'  | 69:AT:52:TRP:CZ3   | 2.51                     | 0.55              |
| 61:B2:1900:U:H2'  | 61:B2:1901:A:H8    | 1.72                     | 0.55              |
| 62:A5:1402:U:OP1  | 62:A5:1510:G:N2    | 2.40                     | 0.55              |
| 70:AF:141:ILE:O   | 70:AF:146:ARG:NH1  | 2.40                     | 0.55              |
| 75:AI:78:ILE:HA   | 75:AI:104:ILE:HG23 | 1.87                     | 0.55              |
| 83:Cj:22:CYS:HG   | 83:Cj:37:CYS:HG    | 1.52                     | 0.55              |
| 12:AS:22:GLY:O    | 12:AS:55:ARG:NH2   | 2.40                     | 0.55              |
| 12:AS:40:TYR:HA   | 12:AS:43:ILE:HB    | 1.88                     | 0.55              |
| 28:CN:96:ARG:NH1  | 28:CN:100:SER:O    | 2.39                     | 0.55              |
| 33:CS:80:ILE:HG22 | 33:CS:129:VAL:HG22 | 1.88                     | 0.55              |
| 47:Ck:28:ASN:ND2  | 62:A5:2063:A:OP2   | 2.36                     | 0.55              |
| 48:Cl:8:ARG:HH22  | 83:Cj:20:ARG:NE    | 2.01                     | 0.55              |
| 61:B2:1251:A:O3'  | 70:AF:169:ARG:NH2  | 2.40                     | 0.55              |
| 62:A5:1986:G:N2   | 62:A5:2086:U:O2    | 2.36                     | 0.55              |
| 62:A5:2131:C:H2'  | 62:A5:2132:A:H4'   | 1.89                     | 0.55              |
| 62:A5:3431:C:O2'  | 62:A5:3433:A:OP2   | 2.25                     | 0.55              |
| 62:A5:3924:U:HO2' | 62:A5:3925:G:N2    | 2.05                     | 0.55              |
| 74:AH:30:GLU:O    | 74:AH:36:LYS:NZ    | 2.36                     | 0.55              |
| 78:CL:79:GLU:OE2  | 78:CL:112:ASN:ND2  | 2.37                     | 0.55              |
| 83:Cj:15:THR:O    | 83:Cj:15:THR:OG1   | 2.25                     | 0.55              |
| 4:CB:244:THR:HG23 | 62:A5:3479:C:H4'   | 1.89                     | 0.55              |
| 6:CC:127:LEU:HD21 | 6:CC:238:LEU:HB3   | 1.89                     | 0.55              |
| 19:AY:120:GLY:O   | 61:B2:84:A:O2'     | 2.25                     | 0.55              |
| 21:Aa:32:LYS:NZ   | 61:B2:1017:A:OP2   | 2.35                     | 0.55              |
| 33:CS:85:ASP:HB2  | 33:CS:123:SER:HB3  | 1.89                     | 0.55              |
| 35:CP:181:LYS:NZ  | 62:A5:3777:U:O5'   | 2.39                     | 0.55              |
| 40:Ch:5:LYS:NZ    | 59:A8:85:G:O5'     | 2.38                     | 0.55              |
| 44:Ce:61:SER:OG   | 44:Ce:62:ASN:N     | 2.39                     | 0.55              |
| 55:CE:20:HIS:ND1  | 55:CE:31:LEU:O     | 2.40                     | 0.55              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 61:B2:51:A:OP2    | 61:B2:429:C:N4     | 2.40                     | 0.55              |
| 61:B2:307:U:OP1   | 75:AI:22:ARG:NH2   | 2.39                     | 0.55              |
| 62:A5:342:A:N7    | 62:A5:343:A:N6     | 2.54                     | 0.55              |
| 62:A5:803:A:O2'   | 62:A5:1684:G:N2    | 2.40                     | 0.55              |
| 62:A5:3544:G:OP1  | 77:CO:63:ARG:NH1   | 2.40                     | 0.55              |
| 62:A5:3760:A:OP1  | 80:CM:101:ARG:NH1  | 2.40                     | 0.55              |
| 1:AA:85:ARG:O     | 1:AA:85:ARG:NH1    | 2.36                     | 0.54              |
| 23:AD:56:LYS:HD2  | 23:AD:58:GLN:HE22  | 1.72                     | 0.54              |
| 29:CI:86:HIS:HB3  | 29:CI:139:ARG:HB3  | 1.88                     | 0.54              |
| 39:Cr:69:LYS:HE3  | 39:Cr:70:LYS:HZ2   | 1.72                     | 0.54              |
| 46:CI:92:ARG:HH11 | 62:A5:313:A:H1'    | 1.71                     | 0.54              |
| 55:CE:200:LYS:HA  | 55:CE:203:LYS:HD2  | 1.88                     | 0.54              |
| 61:B2:950:U:OP1   | 64:AW:28:ARG:NH1   | 2.40                     | 0.54              |
| 62:A5:1106:A:OP1  | 62:A5:1794:G:O2'   | 2.25                     | 0.54              |
| 62:A5:3356:G:O6   | 62:A5:3396:A:N6    | 2.40                     | 0.54              |
| 77:CO:22:ALA:HA   | 77:CO:25:VAL:HG12  | 1.88                     | 0.54              |
| 80:CM:130:LEU:O   | 80:CM:135:LYS:NZ   | 2.32                     | 0.54              |
| 2:CA:5:ILE:HG21   | 2:CA:210:PRO:HD3   | 1.87                     | 0.54              |
| 2:CA:6:ARG:NH2    | 62:A5:2562:U:OP1   | 2.40                     | 0.54              |
| 4:CB:152:LYS:NZ   | 62:A5:3809:U:O4    | 2.40                     | 0.54              |
| 4:CB:248:LEU:N    | 62:A5:2205:G:OP1   | 2.39                     | 0.54              |
| 18:AV:46:GLN:NE2  | 18:AV:47:THR:O     | 2.40                     | 0.54              |
| 27:Ca:139:LYS:HG2 | 27:Ca:144:VAL:HG12 | 1.89                     | 0.54              |
| 29:CI:61:SER:HA   | 29:CI:126:VAL:HG23 | 1.90                     | 0.54              |
| 29:CI:110:ARG:HD2 | 81:B:72:A:H5''     | 1.88                     | 0.54              |
| 35:CP:23:ARG:NH2  | 35:CP:141:SER:OG   | 2.30                     | 0.54              |
| 37:CY:110:LYS:HE2 | 37:CY:115:ARG:HH12 | 1.73                     | 0.54              |
| 46:CI:85:ARG:NH2  | 62:A5:2594:G:OP2   | 2.33                     | 0.54              |
| 61:B2:713:A:OP1   | 74:AH:104:ARG:NH2  | 2.40                     | 0.54              |
| 61:B2:872:A:N6    | 72:AE:19:MET:SD    | 2.80                     | 0.54              |
| 62:A5:2168:G:N2   | 83:Cj:9:GLY:CA     | 2.70                     | 0.54              |
| 62:A5:2795:U:O2'  | 62:A5:3496:U:O2    | 2.25                     | 0.54              |
| 68:AK:56:VAL:HG23 | 68:AK:69:LEU:HA    | 1.89                     | 0.54              |
| 69:AT:30:VAL:CG1  | 69:AT:31:PRO:CD    | 2.84                     | 0.54              |
| 1:AA:42:ARG:HB3   | 1:AA:46:VAL:HB     | 1.89                     | 0.54              |
| 4:CB:92:TYR:HH    | 62:A5:3538:G:HO2'  | 1.55                     | 0.54              |
| 4:CB:340:SER:OG   | 4:CB:341:LYS:N     | 2.29                     | 0.54              |
| 15:AL:80:GLN:NE2  | 61:B2:349:A:O2'    | 2.40                     | 0.54              |
| 34:CT:56:ALA:HA   | 62:A5:3171:A:H4'   | 1.89                     | 0.54              |
| 35:CP:177:ARG:HG3 | 62:A5:3838:A:H61   | 1.72                     | 0.54              |
| 37:CY:56:GLN:N    | 37:CY:105:LEU:O    | 2.39                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 52:Co:44:LYS:NZ    | 62:A5:48:U:O2      | 2.40                     | 0.54              |
| 60:Cz:131:ALA:HB1  | 60:Cz:133:LYS:HE2  | 1.88                     | 0.54              |
| 62:A5:1554:C:N4    | 62:A5:1555:G:O6    | 2.40                     | 0.54              |
| 62:A5:1594:U:O4    | 62:A5:1596:A:N6    | 2.40                     | 0.54              |
| 62:A5:2605:C:H2'   | 62:A5:2606:A:H8    | 1.72                     | 0.54              |
| 62:A5:2718:U:H2'   | 62:A5:2719:A:H8    | 1.73                     | 0.54              |
| 69:AT:60:ILE:HG21  | 69:AT:64:LEU:CD1   | 2.37                     | 0.54              |
| 78:CL:194:ILE:O    | 78:CL:198:ARG:N    | 2.41                     | 0.54              |
| 5:AC:45:PRO:HG3    | 5:AC:54:ARG:HD2    | 1.89                     | 0.54              |
| 5:AC:244:LEU:HG    | 18:AV:52:THR:HG23  | 1.89                     | 0.54              |
| 6:CC:315:SER:HA    | 62:A5:750:G:H4'    | 1.88                     | 0.54              |
| 6:CC:376:LYS:O     | 6:CC:380:ASN:N     | 2.40                     | 0.54              |
| 28:CN:5:ARG:O      | 28:CN:8:GLN:NE2    | 2.39                     | 0.54              |
| 54:CH:103:THR:HG21 | 54:CH:133:VAL:HA   | 1.88                     | 0.54              |
| 55:CE:40:LYS:O     | 55:CE:42:ARG:NE    | 2.40                     | 0.54              |
| 61:B2:1540:G:H5'   | 69:AT:7:LYS:NZ     | 2.21                     | 0.54              |
| 62:A5:834:G:OP2    | 78:CL:27:GLN:NE2   | 2.32                     | 0.54              |
| 62:A5:2563:G:O2'   | 62:A5:2692:U:OP2   | 2.24                     | 0.54              |
| 62:A5:3463:U:H5''  | 79:CV:43:HIS:CD2   | 2.42                     | 0.54              |
| 62:A5:3502:A:N6    | 81:B:73:C:OP1      | 2.40                     | 0.54              |
| 62:A5:3925:G:H3'   | 62:A5:3926:C:H2'   | 1.90                     | 0.54              |
| 70:AF:144:GLY:O    | 70:AF:146:ARG:NH1  | 2.40                     | 0.54              |
| 71:CF:35:GLU:O     | 71:CF:39:ARG:N     | 2.40                     | 0.54              |
| 72:AE:51:ARG:O     | 72:AE:53:LYS:NZ    | 2.36                     | 0.54              |
| 2:CA:130:SER:OG    | 62:A5:2557:C:O2'   | 2.25                     | 0.54              |
| 4:CB:317:MET:HB3   | 4:CB:382:PRO:HD3   | 1.88                     | 0.54              |
| 6:CC:13:TYR:O      | 6:CC:158:SER:N     | 2.40                     | 0.54              |
| 6:CC:136:VAL:HG22  | 39:Cr:3:THR:HG22   | 1.89                     | 0.54              |
| 7:Ag:173:ARG:HA    | 7:Ag:195:TYR:HA    | 1.90                     | 0.54              |
| 18:AV:15:ARG:NH2   | 18:AV:31:SER:OG    | 2.39                     | 0.54              |
| 20:AZ:66:LEU:HD11  | 70:AF:127:LEU:HD21 | 1.89                     | 0.54              |
| 23:AD:143:LYS:HA   | 23:AD:149:ALA:HA   | 1.90                     | 0.54              |
| 27:Ca:8:LYS:NZ     | 62:A5:995:G:OP1    | 2.33                     | 0.54              |
| 38:CZ:53:VAL:H     | 56:CG:36:LEU:HD21  | 1.73                     | 0.54              |
| 43:Cd:84:ARG:NH1   | 43:Cd:104:THR:OG1  | 2.40                     | 0.54              |
| 44:Ce:57:ILE:HG12  | 62:A5:1147:U:H5''  | 1.88                     | 0.54              |
| 47:Ck:33:LYS:NZ    | 62:A5:2061:G:OP2   | 2.36                     | 0.54              |
| 54:CH:1:MET:O      | 80:CM:33:GLN:NE2   | 2.40                     | 0.54              |
| 55:CE:232:LEU:HD11 | 55:CE:236:GLN:HG2  | 1.90                     | 0.54              |
| 61:B2:1105:U:H2'   | 61:B2:1106:A:H8    | 1.72                     | 0.54              |
| 61:B2:1445:A:C4'   | 69:AT:133:ARG:HH12 | 2.17                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 61:B2:1680:G:H3'   | 61:B2:1707:A:H61   | 1.72                     | 0.54              |
| 61:B2:1727:U:N1    | 70:AF:190:ILE:CG1  | 2.71                     | 0.54              |
| 62:A5:133:U:H3     | 62:A5:145:A:H61    | 1.56                     | 0.54              |
| 62:A5:376:G:N2     | 62:A5:379:A:OP2    | 2.35                     | 0.54              |
| 62:A5:1746:A:H2'   | 62:A5:1747:A:C8    | 2.42                     | 0.54              |
| 69:AT:29:LYS:CE    | 69:AT:106:ALA:CA   | 2.73                     | 0.54              |
| 77:CO:180:THR:HG22 | 80:CM:127:PHE:HZ   | 1.73                     | 0.54              |
| 3:AB:128:VAL:HG11  | 3:AB:175:ILE:HG21  | 1.89                     | 0.54              |
| 6:CC:329:ILE:HD12  | 6:CC:333:PRO:HA    | 1.88                     | 0.54              |
| 8:AU:58:MET:HB2    | 8:AU:88:LYS:HB2    | 1.89                     | 0.54              |
| 28:CN:194:ARG:NH1  | 62:A5:104:A:OP1    | 2.41                     | 0.54              |
| 31:CQ:50:ARG:NH1   | 31:CQ:140:GLN:OE1  | 2.41                     | 0.54              |
| 33:CS:153:PRO:HB3  | 80:CM:6:PHE:HD1    | 1.72                     | 0.54              |
| 36:CX:179:PRO:HA   | 62:A5:20:A:H5''    | 1.89                     | 0.54              |
| 40:Ch:101:ASN:O    | 40:Ch:103:LYS:NZ   | 2.39                     | 0.54              |
| 61:B2:121:A:H4'    | 72:AE:77:ARG:HH12  | 1.73                     | 0.54              |
| 61:B2:1189:G:OP2   | 64:AW:12:LYS:NZ    | 2.38                     | 0.54              |
| 61:B2:1670:G:N2    | 61:B2:1721:C:O2    | 2.41                     | 0.54              |
| 61:B2:1727:U:C4    | 70:AF:190:ILE:CB   | 2.91                     | 0.54              |
| 62:A5:2098:C:OP1   | 66:Cg:38:ASN:ND2   | 2.30                     | 0.54              |
| 69:AT:72:VAL:HG12  | 69:AT:101:ARG:NE   | 1.91                     | 0.54              |
| 71:CF:134:ASN:OD1  | 71:CF:137:ARG:NH1  | 2.39                     | 0.54              |
| 71:CF:196:HIS:O    | 71:CF:200:THR:OG1  | 2.24                     | 0.54              |
| 79:CV:85:ARG:NH2   | 79:CV:100:ASP:OD1  | 2.40                     | 0.54              |
| 1:AA:10:LEU:HD22   | 1:AA:55:TRP:HB3    | 1.89                     | 0.54              |
| 2:CA:20:VAL:HG12   | 2:CA:23:ARG:HE     | 1.71                     | 0.54              |
| 15:AL:108:VAL:HG12 | 15:AL:137:PHE:HB2  | 1.90                     | 0.54              |
| 15:AL:131:LEU:HB2  | 15:AL:135:VAL:HB   | 1.89                     | 0.54              |
| 18:AV:36:VAL:O     | 18:AV:50:SER:OG    | 2.26                     | 0.54              |
| 28:CN:116:LEU:HD13 | 28:CN:135:ILE:HD11 | 1.90                     | 0.54              |
| 35:CP:43:ARG:NH2   | 62:A5:3966:U:O3'   | 2.37                     | 0.54              |
| 39:Cr:94:LEU:O     | 39:Cr:98:LYS:NZ    | 2.39                     | 0.54              |
| 44:Ce:23:GLN:HG3   | 44:Ce:26:ARG:HH11  | 1.73                     | 0.54              |
| 55:CE:184:ILE:HD11 | 55:CE:188:LYS:HD3  | 1.89                     | 0.54              |
| 57:A9:24:G:N2      | 62:A5:3117:A:OP2   | 2.41                     | 0.54              |
| 61:B2:303:C:H5''   | 72:AE:38:LEU:HB2   | 1.90                     | 0.54              |
| 61:B2:1727:U:N3    | 70:AF:190:ILE:CB   | 2.71                     | 0.54              |
| 62:A5:67:A:N3      | 62:A5:82:U:O2'     | 2.40                     | 0.54              |
| 62:A5:73:U:H3'     | 62:A5:74:A:H8      | 1.71                     | 0.54              |
| 62:A5:615:C:H2'    | 62:A5:616:A:H8     | 1.72                     | 0.54              |
| 62:A5:1876:G:OP2   | 66:Cg:58:ARG:NH2   | 2.40                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 62:A5:1980:G:H2'   | 62:A5:1981:A:H8    | 1.72                     | 0.54              |
| 63:Ac:40:ARG:HD3   | 63:Ac:60:GLU:HB3   | 1.90                     | 0.54              |
| 74:AH:176:LYS:NZ   | 74:AH:180:GLY:O    | 2.41                     | 0.54              |
| 2:CA:196:TRP:HB2   | 2:CA:198:LYS:HA    | 1.90                     | 0.54              |
| 10:AX:102:VAL:HG22 | 10:AX:122:VAL:HG12 | 1.88                     | 0.54              |
| 15:AL:124:THR:HG23 | 15:AL:140:LEU:HB2  | 1.89                     | 0.54              |
| 18:AV:67:ASP:HA    | 18:AV:70:LEU:HD13  | 1.90                     | 0.54              |
| 23:AD:24:ASN:N     | 23:AD:24:ASN:OD1   | 2.40                     | 0.54              |
| 29:CI:174:THR:HG23 | 29:CI:176:TYR:H    | 1.73                     | 0.54              |
| 31:CQ:124:ASP:N    | 31:CQ:124:ASP:OD1  | 2.39                     | 0.54              |
| 46:CI:56:GLU:O     | 56:CG:239:ARG:NH1  | 2.41                     | 0.54              |
| 46:CI:78:ARG:NH1   | 62:A5:2596:G:OP2   | 2.40                     | 0.54              |
| 59:A8:26:U:O2      | 62:A5:355:G:N2     | 2.41                     | 0.54              |
| 61:B2:388:G:OP1    | 72:AE:6:LYS:NZ     | 2.41                     | 0.54              |
| 61:B2:439:G:O2'    | 61:B2:441:A:N6     | 2.39                     | 0.54              |
| 62:A5:73:U:O2'     | 62:A5:105:A:O2'    | 2.25                     | 0.54              |
| 62:A5:274:A:N6     | 62:A5:275:U:O2     | 2.41                     | 0.54              |
| 62:A5:458:A:N6     | 62:A5:762:G:OP1    | 2.41                     | 0.54              |
| 62:A5:667:U:H1'    | 62:A5:669:U:H4'    | 1.88                     | 0.54              |
| 62:A5:2213:G:H1    | 62:A5:2717:C:N4    | 2.06                     | 0.54              |
| 62:A5:2746:A:H2'   | 62:A5:2747:G:C8    | 2.43                     | 0.54              |
| 62:A5:3262:A:N1    | 62:A5:3331:A:N6    | 2.55                     | 0.54              |
| 62:A5:3769:C:O3'   | 80:CM:117:ARG:NH1  | 2.41                     | 0.54              |
| 1:AA:183:LEU:HA    | 1:AA:187:GLY:HA3   | 1.88                     | 0.54              |
| 2:CA:113:ILE:HG22  | 2:CA:166:VAL:HA    | 1.89                     | 0.54              |
| 10:AX:28:LYS:NZ    | 61:B2:1220:A:OP1   | 2.40                     | 0.54              |
| 10:AX:107:ARG:NH2  | 61:B2:18:C:O2'     | 2.41                     | 0.54              |
| 31:CQ:13:VAL:HG23  | 31:CQ:14:ARG:HG3   | 1.89                     | 0.54              |
| 31:CQ:62:SER:OG    | 62:A5:985:G:N2     | 2.41                     | 0.54              |
| 37:CY:57:VAL:HA    | 37:CY:104:VAL:HG12 | 1.89                     | 0.54              |
| 41:Cb:44:ARG:NH2   | 62:A5:918:G:OP1    | 2.38                     | 0.54              |
| 55:CE:123:LEU:HB3  | 55:CE:139:ARG:HD2  | 1.90                     | 0.54              |
| 56:CG:143:ALA:HB3  | 56:CG:201:ARG:HH22 | 1.73                     | 0.54              |
| 60:Cz:175:LYS:HG3  | 60:Cz:177:ASP:H    | 1.72                     | 0.54              |
| 61:B2:909:U:N3     | 61:B2:935:A:O2'    | 2.38                     | 0.54              |
| 62:A5:87:U:H2'     | 62:A5:88:U:H6      | 1.73                     | 0.54              |
| 62:A5:2704:A:N6    | 62:A5:2705:U:O4    | 2.41                     | 0.54              |
| 66:Cg:66:SER:H     | 66:Cg:69:LEU:HD12  | 1.73                     | 0.54              |
| 66:Cg:85:LEU:HD12  | 66:Cg:88:ARG:HB3   | 1.89                     | 0.54              |
| 77:CO:46:SER:OG    | 77:CO:47:GLY:N     | 2.41                     | 0.54              |
| 77:CO:196:LYS:O    | 77:CO:200:SER:OG   | 2.24                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 18:AV:16:LYS:NZ    | 18:AV:21:ASN:O     | 2.41                     | 0.54              |
| 30:CD:32:ALA:O     | 30:CD:36:LEU:N     | 2.41                     | 0.54              |
| 54:CH:101:CYS:HA   | 54:CH:112:ILE:HG22 | 1.89                     | 0.54              |
| 59:A8:107:U:O2'    | 59:A8:109:U:O2     | 2.22                     | 0.54              |
| 61:B2:1209:U:H2'   | 61:B2:1210:G:H8    | 1.73                     | 0.54              |
| 61:B2:1727:U:C6    | 70:AF:190:ILE:CG1  | 2.91                     | 0.54              |
| 62:A5:718:U:OP1    | 71:CF:81:ARG:NH1   | 2.41                     | 0.54              |
| 62:A5:1017:A:N7    | 83:Cj:15:THR:CG2   | 2.53                     | 0.54              |
| 62:A5:1450:U:H4'   | 62:A5:1451:G:H5'   | 1.90                     | 0.54              |
| 62:A5:1785:G:N2    | 62:A5:1786:G:O2'   | 2.41                     | 0.54              |
| 4:CB:92:TYR:OH     | 62:A5:3538:G:O2'   | 2.26                     | 0.53              |
| 6:CC:98:MET:O      | 62:A5:808:G:N2     | 2.41                     | 0.53              |
| 10:AX:72:VAL:HB    | 10:AX:81:ILE:HB    | 1.90                     | 0.53              |
| 28:CN:183:THR:OG1  | 28:CN:183:THR:O    | 2.24                     | 0.53              |
| 32:CR:194:ILE:HA   | 32:CR:197:LYS:HE2  | 1.90                     | 0.53              |
| 34:CT:45:HIS:CD2   | 34:CT:94:GLU:O     | 2.60                     | 0.53              |
| 38:CZ:114:ARG:HH22 | 62:A5:1941:A:H4'   | 1.73                     | 0.53              |
| 52:Co:52:THR:OG1   | 52:Co:53:LYS:N     | 2.37                     | 0.53              |
| 56:CG:108:ARG:HH21 | 56:CG:200:ARG:HH11 | 1.55                     | 0.53              |
| 61:B2:713:A:N6     | 74:AH:110:LEU:O    | 2.41                     | 0.53              |
| 61:B2:1733:G:H21   | 61:B2:1762:A:H62   | 1.57                     | 0.53              |
| 61:B2:1782:G:H4'   | 69:AT:92:PHE:CE2   | 2.43                     | 0.53              |
| 61:B2:1938:U:H2'   | 61:B2:1939:A:H8    | 1.73                     | 0.53              |
| 62:A5:1211:A:H61   | 62:A5:1263:U:H3    | 1.54                     | 0.53              |
| 62:A5:1694:A:O2'   | 62:A5:2724:C:O2'   | 2.25                     | 0.53              |
| 62:A5:2220:C:N4    | 62:A5:2221:G:O6    | 2.41                     | 0.53              |
| 62:A5:3196:C:N4    | 62:A5:3235:A:O2'   | 2.41                     | 0.53              |
| 62:A5:3261:U:H2'   | 62:A5:3262:A:H8    | 1.73                     | 0.53              |
| 64:AW:42:MET:HE3   | 64:AW:45:GLY:HA2   | 1.90                     | 0.53              |
| 67:CU:260:LYS:O    | 67:CU:269:ARG:NH2  | 2.41                     | 0.53              |
| 69:AT:23:LYS:HA    | 69:AT:28:LEU:HD21  | 1.88                     | 0.53              |
| 73:AG:48:TYR:OH    | 73:AG:119:LYS:O    | 2.25                     | 0.53              |
| 6:CC:204:ARG:HG2   | 6:CC:205:ILE:HG12  | 1.91                     | 0.53              |
| 17:AP:58:ALA:HA    | 17:AP:61:LYS:HB2   | 1.89                     | 0.53              |
| 21:Aa:94:ILE:HD12  | 21:Aa:97:PRO:HG2   | 1.91                     | 0.53              |
| 25:Af:144:CYS:SG   | 25:Af:147:THR:OG1  | 2.63                     | 0.53              |
| 27:Ca:123:VAL:H    | 27:Ca:143:GLY:HA3  | 1.73                     | 0.53              |
| 29:CI:173:PHE:O    | 29:CI:175:LYS:NZ   | 2.41                     | 0.53              |
| 40:Ch:89:ARG:NH1   | 59:A8:36:A:OP2     | 2.41                     | 0.53              |
| 53:CJ:100:ARG:NE   | 53:CJ:182:THR:OG1  | 2.39                     | 0.53              |
| 62:A5:245:G:OP1    | 62:A5:247:C:N4     | 2.38                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 62:A5:495:A:N6     | 62:A5:504:A:N1     | 2.56                     | 0.53              |
| 62:A5:1311:U:H2'   | 62:A5:1312:G:C8    | 2.36                     | 0.53              |
| 72:AE:249:ALA:HA   | 72:AE:252:ARG:HE   | 1.71                     | 0.53              |
| 1:AA:154:LEU:HA    | 1:AA:157:ILE:HD12  | 1.89                     | 0.53              |
| 5:AC:208:SER:OG    | 5:AC:209:ALA:N     | 2.41                     | 0.53              |
| 9:AO:80:ASP:N      | 9:AO:80:ASP:OD1    | 2.41                     | 0.53              |
| 10:AX:47:ALA:HB1   | 10:AX:74:LEU:HD11  | 1.90                     | 0.53              |
| 16:AR:36:GLU:HB2   | 16:AR:47:ARG:HH22  | 1.73                     | 0.53              |
| 26:AJ:170:ARG:HE   | 26:AJ:173:ARG:HG3  | 1.73                     | 0.53              |
| 29:CI:16:PRO:HG2   | 62:A5:1260:A:H5''  | 1.89                     | 0.53              |
| 34:CT:87:LYS:NZ    | 62:A5:3256:U:OP2   | 2.34                     | 0.53              |
| 39:Cr:51:LYS:HA    | 39:Cr:70:LYS:HD2   | 1.90                     | 0.53              |
| 39:Cr:134:LYS:NZ   | 62:A5:764:A:OP2    | 2.42                     | 0.53              |
| 44:Ce:75:LYS:NZ    | 62:A5:1651:C:O2    | 2.38                     | 0.53              |
| 55:CE:220:LYS:HZ3  | 80:CM:109:ARG:HB3  | 1.71                     | 0.53              |
| 56:CG:110:GLU:O    | 56:CG:200:ARG:NH2  | 2.41                     | 0.53              |
| 61:B2:1540:G:N2    | 69:AT:129:ARG:NE   | 2.55                     | 0.53              |
| 62:A5:1381:U:O2    | 62:A5:1382:U:N3    | 2.42                     | 0.53              |
| 62:A5:1499:C:H3'   | 62:A5:1500:G:H21   | 1.74                     | 0.53              |
| 62:A5:2836:A:N6    | 62:A5:2881:U:O2'   | 2.40                     | 0.53              |
| 62:A5:3132:C:H2'   | 62:A5:3133:A:H8    | 1.74                     | 0.53              |
| 70:AF:101:MET:HB3  | 70:AF:107:ASN:HA   | 1.89                     | 0.53              |
| 74:AH:131:LEU:HD23 | 74:AH:132:VAL:HG13 | 1.89                     | 0.53              |
| 80:CM:6:PHE:O      | 80:CM:11:ARG:NH1   | 2.41                     | 0.53              |
| 4:CB:226:LYS:NZ    | 62:A5:3624:C:O3'   | 2.42                     | 0.53              |
| 6:CC:97:ASN:HD21   | 62:A5:1003:C:H4'   | 1.73                     | 0.53              |
| 17:AP:46:ARG:NH1   | 61:B2:1745:G:O6    | 2.42                     | 0.53              |
| 27:Ca:23:ILE:HD12  | 62:A5:1328:U:H5''  | 1.90                     | 0.53              |
| 28:CN:176:LYS:NZ   | 62:A5:81:A:O3'     | 2.41                     | 0.53              |
| 34:CT:142:LYS:HG3  | 34:CT:144:LEU:HB3  | 1.90                     | 0.53              |
| 60:Cz:68:LEU:HD12  | 60:Cz:112:ALA:HA   | 1.89                     | 0.53              |
| 61:B2:1668:A:OP2   | 69:AT:84:ARG:HD2   | 2.07                     | 0.53              |
| 61:B2:1885:U:H2'   | 61:B2:1886:G:H8    | 1.74                     | 0.53              |
| 62:A5:378:G:H21    | 62:A5:1015:G:H1'   | 1.74                     | 0.53              |
| 62:A5:1954:G:O2'   | 62:A5:1955:A:O4'   | 2.26                     | 0.53              |
| 62:A5:3721:C:N4    | 62:A5:3761:U:O4    | 2.41                     | 0.53              |
| 62:A5:3926:C:H42   | 75:AI:128:LYS:HB2  | 1.73                     | 0.53              |
| 75:AI:132:LYS:HB3  | 75:AI:135:GLU:H    | 1.73                     | 0.53              |
| 77:CO:195:ASN:HA   | 77:CO:198:ILE:HG22 | 1.91                     | 0.53              |
| 5:AC:242:MET:HB3   | 5:AC:244:LEU:H     | 1.73                     | 0.53              |
| 6:CC:66:SER:HB2    | 62:A5:1129:A:H5''  | 1.90                     | 0.53              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 9:AO:91:THR:OG1   | 9:AO:125:LYS:NZ    | 2.41                     | 0.53              |
| 13:Ad:16:GLN:HE22 | 13:Ad:27:ARG:NH2   | 2.05                     | 0.53              |
| 58:A7:103:A:O2'   | 62:A5:1214:G:O6    | 2.27                     | 0.53              |
| 61:B2:1696:G:N1   | 61:B2:1741:A:O2'   | 2.41                     | 0.53              |
| 62:A5:108:A:H2'   | 62:A5:109:A:H8     | 1.74                     | 0.53              |
| 62:A5:2019:U:H3   | 62:A5:2052:G:H22   | 1.55                     | 0.53              |
| 70:AF:81:ALA:HA   | 70:AF:86:ARG:HG3   | 1.90                     | 0.53              |
| 73:AG:50:LEU:HD21 | 73:AG:111:LEU:HB3  | 1.90                     | 0.53              |
| 1:AA:54:THR:HA    | 1:AA:57:LYS:HG2    | 1.90                     | 0.53              |
| 4:CB:374:MET:O    | 62:A5:3621:A:O2'   | 2.27                     | 0.53              |
| 10:AX:88:ASP:HB3  | 61:B2:576:G:H4'    | 1.90                     | 0.53              |
| 15:AL:9:PHE:N     | 75:AI:200:TYR:OH   | 2.41                     | 0.53              |
| 15:AL:35:ARG:NH1  | 15:AL:61:GLY:O     | 2.42                     | 0.53              |
| 19:AY:90:TYR:HB3  | 61:B2:533:A:H4'    | 1.89                     | 0.53              |
| 20:AZ:57:LEU:HA   | 20:AZ:60:GLU:HB2   | 1.90                     | 0.53              |
| 27:Ca:115:ARG:NH1 | 62:A5:855:A:OP1    | 2.42                     | 0.53              |
| 28:CN:146:PRO:HA  | 28:CN:149:ASN:HB2  | 1.90                     | 0.53              |
| 42:Cc:21:VAL:O    | 42:Cc:25:GLY:N     | 2.39                     | 0.53              |
| 51:Cp:17:ARG:HH12 | 62:A5:1060:G:H5''  | 1.73                     | 0.53              |
| 61:B2:663:A:H5''  | 61:B2:690:U:H5'    | 1.91                     | 0.53              |
| 62:A5:50:U:H2'    | 62:A5:51:U:H6      | 1.74                     | 0.53              |
| 62:A5:285:G:O5'   | 62:A5:336:A:N6     | 2.42                     | 0.53              |
| 62:A5:595:U:H3    | 62:A5:614:G:H22    | 1.57                     | 0.53              |
| 62:A5:3293:G:N3   | 62:A5:3332:G:N2    | 2.56                     | 0.53              |
| 69:AT:19:ALA:O    | 69:AT:23:LYS:HG3   | 2.07                     | 0.53              |
| 73:AG:183:PRO:HA  | 73:AG:186:LEU:HD23 | 1.91                     | 0.53              |
| 1:AA:151:ASP:N    | 1:AA:151:ASP:OD1   | 2.37                     | 0.53              |
| 3:AB:103:PHE:HB3  | 3:AB:184:LEU:HD11  | 1.91                     | 0.53              |
| 3:AB:173:ASP:OD1  | 3:AB:173:ASP:N     | 2.37                     | 0.53              |
| 9:AO:143:LYS:HZ1  | 61:B2:1095:G:H5''  | 1.73                     | 0.53              |
| 26:AJ:76:ASN:HA   | 26:AJ:79:LEU:HD12  | 1.91                     | 0.53              |
| 28:CN:124:ASP:O   | 28:CN:126:SER:N    | 2.40                     | 0.53              |
| 32:CR:169:ALA:O   | 32:CR:172:ARG:NH1  | 2.42                     | 0.53              |
| 37:CY:21:ALA:O    | 37:CY:26:ARG:NH1   | 2.41                     | 0.53              |
| 61:B2:912:U:O4    | 61:B2:931:A:N6     | 2.41                     | 0.53              |
| 62:A5:475:U:O2    | 62:A5:477:C:N4     | 2.37                     | 0.53              |
| 62:A5:1470:C:N4   | 62:A5:1477:G:OP2   | 2.41                     | 0.53              |
| 62:A5:2485:A:H2'  | 62:A5:2486:A:H8    | 1.73                     | 0.53              |
| 7:Ag:32:ILE:HB    | 7:Ag:40:LEU:HD11   | 1.91                     | 0.53              |
| 7:Ag:196:LEU:HA   | 7:Ag:212:GLY:HA2   | 1.91                     | 0.53              |
| 28:CN:198:GLU:HB2 | 78:CL:21:VAL:HG22  | 1.90                     | 0.53              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 29:CI:196:ASN:N   | 29:CI:196:ASN:ND2  | 2.57                     | 0.53              |
| 31:CQ:165:PRO:HG3 | 31:CQ:180:ARG:HH22 | 1.72                     | 0.53              |
| 33:CS:36:ASP:HB3  | 33:CS:38:ILE:HG22  | 1.91                     | 0.53              |
| 34:CT:129:LYS:HE2 | 62:A5:1310:A:H5'   | 1.90                     | 0.53              |
| 61:B2:1012:G:H2'  | 61:B2:1013:A:H8    | 1.74                     | 0.53              |
| 61:B2:1441:C:N3   | 61:B2:1543:G:N2    | 2.53                     | 0.53              |
| 61:B2:1727:U:C5   | 70:AF:190:ILE:CG1  | 2.92                     | 0.53              |
| 62:A5:330:C:H2'   | 62:A5:331:A:H8     | 1.73                     | 0.53              |
| 62:A5:2577:G:H1   | 62:A5:2623:C:H42   | 1.55                     | 0.53              |
| 62:A5:3244:U:HO2' | 62:A5:3275:G:HO2'  | 1.52                     | 0.53              |
| 62:A5:3600:G:H2'  | 62:A5:3601:U:H6    | 1.74                     | 0.53              |
| 69:AT:17:ALA:O    | 69:AT:21:PHE:HD2   | 1.82                     | 0.53              |
| 71:CF:38:ARG:HA   | 71:CF:41:LYS:HB2   | 1.90                     | 0.53              |
| 74:AH:169:ASP:N   | 74:AH:169:ASP:OD1  | 2.40                     | 0.53              |
| 75:AI:146:LYS:O   | 75:AI:150:LYS:N    | 2.41                     | 0.53              |
| 77:CO:181:VAL:HA  | 77:CO:184:ARG:HB2  | 1.90                     | 0.53              |
| 2:CA:113:ILE:HA   | 2:CA:167:GLY:H     | 1.74                     | 0.53              |
| 2:CA:200:ARG:NH2  | 62:A5:2525:C:OP1   | 2.41                     | 0.53              |
| 2:CA:207:VAL:HG21 | 62:A5:1116:G:C6    | 2.44                     | 0.53              |
| 6:CC:48:ARG:HH21  | 62:A5:356:A:H62    | 1.57                     | 0.53              |
| 10:AX:68:LYS:NZ   | 61:B2:576:G:OP2    | 2.41                     | 0.53              |
| 16:AR:57:LEU:O    | 16:AR:61:LEU:N     | 2.39                     | 0.53              |
| 27:Ca:17:SER:OG   | 62:A5:1611:G:OP1   | 2.19                     | 0.53              |
| 27:Ca:97:THR:OG1  | 27:Ca:98:LYS:NZ    | 2.42                     | 0.53              |
| 35:CP:31:GLU:OE1  | 35:CP:63:PHE:N     | 2.34                     | 0.53              |
| 45:Cf:155:SER:OG  | 45:Cf:156:ARG:N    | 2.40                     | 0.53              |
| 56:CG:169:LEU:O   | 56:CG:173:LEU:N    | 2.42                     | 0.53              |
| 61:B2:65:A:OP2    | 73:AG:178:GLN:NE2  | 2.39                     | 0.53              |
| 62:A5:203:A:O2'   | 62:A5:229:C:O2'    | 2.25                     | 0.53              |
| 62:A5:2177:G:O2'  | 62:A5:3601:U:OP1   | 2.27                     | 0.53              |
| 69:AT:72:VAL:CB   | 69:AT:101:ARG:HG2  | 2.37                     | 0.53              |
| 74:AH:60:ILE:HB   | 74:AH:92:VAL:HA    | 1.91                     | 0.53              |
| 78:CL:55:ARG:NE   | 78:CL:72:GLY:O     | 2.42                     | 0.53              |
| 2:CA:104:LEU:HD23 | 2:CA:107:MET:HE3   | 1.91                     | 0.53              |
| 4:CB:223:THR:OG1  | 4:CB:224:LYS:N     | 2.41                     | 0.53              |
| 6:CC:381:ARG:HD3  | 6:CC:384:LEU:HD12  | 1.91                     | 0.53              |
| 7:Ag:85:ASP:OD2   | 7:Ag:89:ARG:NH2    | 2.38                     | 0.53              |
| 7:Ag:243:SER:OG   | 7:Ag:245:ASN:OD1   | 2.26                     | 0.53              |
| 18:AV:4:ASP:OD1   | 18:AV:4:ASP:N      | 2.38                     | 0.53              |
| 19:AY:17:ARG:HH21 | 19:AY:22:LYS:HG3   | 1.73                     | 0.53              |
| 22:Ab:24:LEU:HD12 | 22:Ab:25:VAL:HG13  | 1.90                     | 0.53              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 24:Ae:97:LYS:NZ    | 61:B2:513:A:OP1   | 2.41                     | 0.53              |
| 27:Ca:11:LYS:HA    | 62:A5:1144:C:H41  | 1.73                     | 0.53              |
| 27:Ca:80:TRP:HA    | 27:Ca:83:VAL:HG22 | 1.91                     | 0.53              |
| 33:CS:89:GLY:O     | 33:CS:91:HIS:ND1  | 2.36                     | 0.53              |
| 61:B2:429:C:O2     | 61:B2:432:C:N4    | 2.41                     | 0.53              |
| 61:B2:1660:U:H1'   | 69:AT:88:HIS:CE1  | 2.43                     | 0.53              |
| 62:A5:298:U:H3     | 62:A5:300:A:H3'   | 1.74                     | 0.53              |
| 62:A5:990:U:H2'    | 62:A5:991:A:H8    | 1.73                     | 0.53              |
| 62:A5:2214:G:OP1   | 79:CV:101:ASN:ND2 | 2.42                     | 0.53              |
| 64:AW:85:ASP:OD1   | 64:AW:85:ASP:N    | 2.36                     | 0.53              |
| 77:CO:15:GLY:O     | 77:CO:127:ARG:N   | 2.42                     | 0.53              |
| 77:CO:112:SER:O    | 77:CO:114:TYR:N   | 2.42                     | 0.53              |
| 83:Cj:20:ARG:HG2   | 83:Cj:20:ARG:NH1  | 2.24                     | 0.53              |
| 2:CA:51:ASP:OD2    | 2:CA:54:ARG:NE    | 2.41                     | 0.52              |
| 14:AN:91:MET:O     | 14:AN:95:ALA:N    | 2.40                     | 0.52              |
| 24:Ae:80:ARG:HG3   | 61:B2:575:A:H5'   | 1.91                     | 0.52              |
| 25:Af:130:VAL:HG21 | 25:Af:141:CYS:HB2 | 1.91                     | 0.52              |
| 29:CI:98:ARG:HH21  | 62:A5:1340:G:H5'' | 1.74                     | 0.52              |
| 33:CS:15:ARG:NH1   | 33:CS:25:THR:OG1  | 2.42                     | 0.52              |
| 46:CI:86:ARG:NH1   | 62:A5:312:U:OP1   | 2.38                     | 0.52              |
| 53:CJ:155:THR:OG1  | 53:CJ:156:VAL:N   | 2.42                     | 0.52              |
| 53:CJ:167:ALA:O    | 53:CJ:171:PHE:N   | 2.41                     | 0.52              |
| 55:CE:85:SER:OG    | 62:A5:755:A:N3    | 2.41                     | 0.52              |
| 60:Cz:72:GLN:HB2   | 60:Cz:144:MET:HE1 | 1.90                     | 0.52              |
| 61:B2:444:U:O5'    | 61:B2:470:G:N2    | 2.42                     | 0.52              |
| 61:B2:630:A:N6     | 61:B2:1119:G:N7   | 2.57                     | 0.52              |
| 62:A5:1273:U:H2'   | 62:A5:1274:A:H8   | 1.73                     | 0.52              |
| 62:A5:1292:G:N3    | 62:A5:1296:U:N3   | 2.56                     | 0.52              |
| 62:A5:3491:C:H2'   | 62:A5:3492:G:H8   | 1.72                     | 0.52              |
| 70:AF:161:GLN:NE2  | 70:AF:227:ASN:O   | 2.41                     | 0.52              |
| 73:AG:102:VAL:HA   | 73:AG:106:MET:HE3 | 1.91                     | 0.52              |
| 75:AI:110:ARG:HH21 | 75:AI:122:GLY:H   | 1.55                     | 0.52              |
| 77:CO:168:VAL:O    | 77:CO:172:HIS:N   | 2.42                     | 0.52              |
| 81:B:20:A:O2'      | 81:B:45:G:O6      | 2.28                     | 0.52              |
| 2:CA:77:ILE:HG12   | 2:CA:128:ARG:HD3  | 1.91                     | 0.52              |
| 2:CA:122:ASP:OD1   | 62:A5:2913:G:O2'  | 2.26                     | 0.52              |
| 4:CB:287:ILE:HG22  | 4:CB:331:VAL:HG12 | 1.91                     | 0.52              |
| 23:AD:137:GLU:HB3  | 23:AD:189:LYS:HB2 | 1.90                     | 0.52              |
| 28:CN:50:ARG:NH1   | 62:A5:286:A:OP2   | 2.40                     | 0.52              |
| 28:CN:54:ARG:NH1   | 62:A5:117:C:O3'   | 2.42                     | 0.52              |
| 34:CT:41:ASP:HA    | 34:CT:61:THR:HA   | 1.91                     | 0.52              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 40:Ch:62:HIS:O    | 40:Ch:66:LYS:N     | 2.41                     | 0.52              |
| 58:A7:69:C:H2'    | 58:A7:70:G:H8      | 1.74                     | 0.52              |
| 61:B2:1004:C:N4   | 61:B2:1005:G:O6    | 2.42                     | 0.52              |
| 61:B2:1828:C:H42  | 61:B2:1962:G:H1    | 1.57                     | 0.52              |
| 61:B2:1881:A:N6   | 61:B2:1900:U:OP1   | 2.43                     | 0.52              |
| 62:A5:1109:G:O6   | 62:A5:1119:C:N4    | 2.43                     | 0.52              |
| 62:A5:1788:G:N2   | 62:A5:1791:A:OP2   | 2.42                     | 0.52              |
| 62:A5:2591:A:H2'  | 62:A5:2592:A:C8    | 2.43                     | 0.52              |
| 62:A5:3815:G:H3'  | 62:A5:3816:A:H8    | 1.73                     | 0.52              |
| 78:CL:15:LYS:H    | 78:CL:17:TRP:CD1   | 2.26                     | 0.52              |
| 3:AB:30:TRP:O     | 3:AB:97:ARG:NH1    | 2.42                     | 0.52              |
| 13:Ad:5:THR:OG1   | 13:Ad:6:LEU:N      | 2.38                     | 0.52              |
| 19:AY:24:MET:HG3  | 19:AY:74:ALA:HB3   | 1.92                     | 0.52              |
| 28:CN:93:LYS:HD2  | 62:A5:295:G:H1'    | 1.92                     | 0.52              |
| 33:CS:118:ARG:O   | 33:CS:120:ARG:NH1  | 2.42                     | 0.52              |
| 36:CX:163:THR:HA  | 56:CG:56:LEU:HB2   | 1.91                     | 0.52              |
| 37:CY:9:SER:O     | 62:A5:236:G:O2'    | 2.26                     | 0.52              |
| 37:CY:100:HIS:CD2 | 37:CY:101:PRO:HD2  | 2.44                     | 0.52              |
| 44:Ce:2:THR:O     | 62:A5:762:G:N2     | 2.42                     | 0.52              |
| 61:B2:334:G:OP1   | 75:AI:99:ASN:ND2   | 2.42                     | 0.52              |
| 62:A5:1172:G:N1   | 62:A5:1322:U:O4    | 2.42                     | 0.52              |
| 69:AT:68:SER:HB2  | 69:AT:69:PRO:HD2   | 1.92                     | 0.52              |
| 69:AT:126:ILE:CG2 | 69:AT:131:LEU:CG   | 2.63                     | 0.52              |
| 71:CF:49:ARG:NE   | 71:CF:179:GLU:OE2  | 2.41                     | 0.52              |
| 2:CA:36:GLU:HG3   | 2:CA:91:GLY:HA2    | 1.92                     | 0.52              |
| 4:CB:16:PHE:O     | 62:A5:3672:U:O2'   | 2.21                     | 0.52              |
| 6:CC:208:ARG:NE   | 62:A5:1624:G:OP1   | 2.42                     | 0.52              |
| 21:Aa:11:ASN:OD1  | 61:B2:1021:A:O2'   | 2.26                     | 0.52              |
| 23:AD:44:THR:O    | 23:AD:85:ARG:NH2   | 2.36                     | 0.52              |
| 30:CD:95:TYR:HD1  | 30:CD:158:ARG:HG2  | 1.75                     | 0.52              |
| 59:A8:56:U:H5     | 83:Cj:63:ARG:HH21  | 1.49                     | 0.52              |
| 61:B2:1811:C:N3   | 63:Ac:20:GLN:NE2   | 2.57                     | 0.52              |
| 62:A5:426:A:N3    | 62:A5:805:C:O2'    | 2.42                     | 0.52              |
| 65:CW:6:CYS:SG    | 65:CW:8:PHE:N      | 2.71                     | 0.52              |
| 69:AT:23:LYS:CB   | 69:AT:28:LEU:CD2   | 2.88                     | 0.52              |
| 80:CM:135:LYS:H   | 80:CM:141:ARG:HH22 | 1.57                     | 0.52              |
| 7:Ag:132:LEU:HB2  | 7:Ag:141:PHE:HB3   | 1.91                     | 0.52              |
| 13:Ad:23:ALA:O    | 68:AK:63:ARG:NH1   | 2.43                     | 0.52              |
| 28:CN:159:ARG:NH2 | 62:A5:339:C:OP1    | 2.42                     | 0.52              |
| 30:CD:36:LEU:O    | 30:CD:48:LYS:NZ    | 2.35                     | 0.52              |
| 32:CR:99:GLN:NE2  | 32:CR:127:CYS:O    | 2.41                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 38:CZ:105:LYS:O    | 38:CZ:108:THR:OG1  | 2.27                     | 0.52              |
| 39:Cr:27:LYS:HD3   | 62:A5:1595:G:C5    | 2.45                     | 0.52              |
| 43:Cd:31:HIS:HB2   | 62:A5:3950:A:N3    | 2.24                     | 0.52              |
| 46:Ci:40:LYS:HG3   | 62:A5:284:A:C4     | 2.44                     | 0.52              |
| 61:B2:861:U:O2'    | 61:B2:864:A:N6     | 2.36                     | 0.52              |
| 61:B2:1638:A:O2'   | 61:B2:1640:G:N7    | 2.39                     | 0.52              |
| 62:A5:918:G:H22    | 62:A5:982:C:H42    | 1.57                     | 0.52              |
| 62:A5:2209:G:N2    | 62:A5:2721:C:O2    | 2.43                     | 0.52              |
| 72:AE:161:GLN:HB3  | 72:AE:171:ASP:HB3  | 1.92                     | 0.52              |
| 73:AG:76:LEU:HG    | 73:AG:94:ARG:HB2   | 1.90                     | 0.52              |
| 76:AQ:29:ARG:HA    | 76:AQ:68:VAL:HA    | 1.92                     | 0.52              |
| 78:CL:67:THR:OG1   | 78:CL:68:LYS:N     | 2.42                     | 0.52              |
| 81:B:15:G:H21      | 81:B:19:A:H61      | 1.56                     | 0.52              |
| 4:CB:19:LYS:HG3    | 4:CB:275:HIS:CE1   | 2.44                     | 0.52              |
| 4:CB:157:CYS:SG    | 4:CB:158:LYS:N     | 2.83                     | 0.52              |
| 14:AN:151:ALA:OXT  | 42:Cc:86:GLY:N     | 2.43                     | 0.52              |
| 15:AL:54:ASP:OD2   | 15:AL:81:ARG:NH1   | 2.42                     | 0.52              |
| 21:Aa:89:ARG:NH1   | 61:B2:1175:A:O3'   | 2.43                     | 0.52              |
| 28:CN:157:LYS:NZ   | 62:A5:61:A:OP1     | 2.42                     | 0.52              |
| 36:CX:260:ARG:NH1  | 62:A5:1893:C:OP1   | 2.42                     | 0.52              |
| 44:Ce:42:ASN:ND2   | 62:A5:789:G:OP1    | 2.43                     | 0.52              |
| 49:Cm:94:MET:HG2   | 49:Cm:105:PRO:HA   | 1.90                     | 0.52              |
| 56:CG:147:THR:N    | 62:A5:156:G:O6     | 2.43                     | 0.52              |
| 61:B2:399:C:H42    | 61:B2:406:A:H62    | 1.56                     | 0.52              |
| 61:B2:450:A:H61    | 61:B2:467:G:H1'    | 1.75                     | 0.52              |
| 61:B2:1513:U:H5''  | 61:B2:1514:G:H5'   | 1.91                     | 0.52              |
| 61:B2:1715:G:N3    | 69:AT:67:ARG:HG2   | 2.24                     | 0.52              |
| 62:A5:93:G:H21     | 62:A5:299:G:H4'    | 1.73                     | 0.52              |
| 62:A5:2477:C:H2'   | 62:A5:2478:A:H8    | 1.73                     | 0.52              |
| 72:AE:36:HIS:CE1   | 72:AE:88:ASP:OD2   | 2.63                     | 0.52              |
| 73:AG:122:PRO:HA   | 73:AG:126:ASP:HB2  | 1.91                     | 0.52              |
| 74:AH:8:ILE:HG13   | 74:AH:26:LEU:HD22  | 1.90                     | 0.52              |
| 76:AQ:32:GLY:HA2   | 76:AQ:69:ASP:HA    | 1.91                     | 0.52              |
| 4:CB:95:THR:OG1    | 4:CB:98:GLY:N      | 2.42                     | 0.52              |
| 8:AU:55:PRO:HB3    | 8:AU:89:ARG:HD3    | 1.91                     | 0.52              |
| 24:Ae:103:ARG:HH12 | 61:B2:483:A:H5'    | 1.74                     | 0.52              |
| 28:CN:33:LEU:HD13  | 28:CN:37:HIS:CE1   | 2.45                     | 0.52              |
| 28:CN:128:LYS:NZ   | 62:A5:309:C:OP2    | 2.35                     | 0.52              |
| 29:CI:44:GLU:HA    | 29:CI:171:TRP:HH2  | 1.75                     | 0.52              |
| 52:Co:19:LYS:HD3   | 52:Co:74:GLU:HG3   | 1.92                     | 0.52              |
| 60:Cz:157:PHE:HB3  | 60:Cz:167:VAL:HG21 | 1.92                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 61:B2:1727:U:N3    | 70:AF:190:ILE:HG12 | 2.24                     | 0.52              |
| 61:B2:1797:G:H5''  | 76:AQ:132:LYS:HB3  | 1.91                     | 0.52              |
| 62:A5:807:A:H2'    | 62:A5:808:G:H8     | 1.75                     | 0.52              |
| 62:A5:1807:U:H3    | 62:A5:1859:U:H3    | 1.58                     | 0.52              |
| 62:A5:2127:C:N4    | 62:A5:2130:G:O2'   | 2.42                     | 0.52              |
| 69:AT:6:VAL:CG1    | 69:AT:136:ASN:OD1  | 2.54                     | 0.52              |
| 71:CF:95:VAL:HG22  | 71:CF:145:TRP:HB3  | 1.92                     | 0.52              |
| 76:AQ:11:ALA:HB2   | 76:AQ:28:LYS:HB3   | 1.91                     | 0.52              |
| 4:CB:71:GLU:HG2    | 4:CB:366:LYS:HE3   | 1.91                     | 0.52              |
| 16:AR:25:THR:HG23  | 16:AR:27:ASP:H     | 1.73                     | 0.52              |
| 23:AD:75:VAL:HA    | 23:AD:78:ARG:HB3   | 1.91                     | 0.52              |
| 26:AJ:22:GLU:HB3   | 26:AJ:25:ARG:HG2   | 1.92                     | 0.52              |
| 32:CR:190:LYS:HA   | 32:CR:193:GLU:HB3  | 1.92                     | 0.52              |
| 34:CT:78:LYS:NZ    | 62:A5:3256:U:OP1   | 2.39                     | 0.52              |
| 45:Cf:46:ARG:HD2   | 55:CE:234:SER:HA   | 1.90                     | 0.52              |
| 61:B2:519:A:N1     | 61:B2:546:A:O2'    | 2.34                     | 0.52              |
| 61:B2:902:A:N6     | 61:B2:939:G:OP2    | 2.42                     | 0.52              |
| 61:B2:1343:A:OP1   | 61:B2:1346:C:N4    | 2.43                     | 0.52              |
| 61:B2:1776:G:O4'   | 76:AQ:127:ARG:NH2  | 2.42                     | 0.52              |
| 62:A5:1796:A:H62   | 62:A5:2552:G:H3'   | 1.75                     | 0.52              |
| 62:A5:3274:A:H2'   | 62:A5:3275:G:H8    | 1.75                     | 0.52              |
| 69:AT:136:ASN:HB3  | 69:AT:140:PHE:CE2  | 2.34                     | 0.52              |
| 77:CO:32:GLY:H     | 77:CO:103:ARG:HH12 | 1.57                     | 0.52              |
| 81:B:3:C:H2'       | 81:B:4:A:H8        | 1.75                     | 0.52              |
| 1:AA:21:ALA:HB2    | 1:AA:173:LEU:HD23  | 1.91                     | 0.52              |
| 3:AB:42:ARG:NH2    | 3:AB:236:GLY:O     | 2.42                     | 0.52              |
| 8:AU:56:VAL:HB     | 8:AU:90:ILE:HB     | 1.92                     | 0.52              |
| 20:AZ:61:VAL:HA    | 20:AZ:64:TYR:HB3   | 1.91                     | 0.52              |
| 22:Ab:7:LEU:H      | 64:AW:24:GLN:HE22  | 1.58                     | 0.52              |
| 23:AD:29:ARG:NH1   | 68:AK:60:PHE:O     | 2.43                     | 0.52              |
| 23:AD:78:ARG:NH1   | 23:AD:78:ARG:O     | 2.42                     | 0.52              |
| 33:CS:132:ILE:HD11 | 33:CS:136:LYS:HB2  | 1.91                     | 0.52              |
| 37:CY:11:ARG:NH2   | 59:A8:21:U:OP1     | 2.37                     | 0.52              |
| 40:Ch:78:TYR:OH    | 62:A5:131:U:OP1    | 2.27                     | 0.52              |
| 44:Ce:82:ARG:NH1   | 44:Ce:85:GLU:OE1   | 2.43                     | 0.52              |
| 46:Ci:76:ASP:OD1   | 46:Ci:76:ASP:N     | 2.42                     | 0.52              |
| 53:CJ:115:GLN:NE2  | 62:A5:3206:A:N3    | 2.57                     | 0.52              |
| 55:CE:71:THR:H     | 55:CE:72:LYS:HG2   | 1.75                     | 0.52              |
| 56:CG:85:ILE:HA    | 56:CG:87:GLN:H     | 1.75                     | 0.52              |
| 60:Cz:97:LYS:HE3   | 62:A5:2874:A:H5''  | 1.92                     | 0.52              |
| 61:B2:1187:U:N3    | 61:B2:1188:G:N7    | 2.58                     | 0.52              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 61:B2:1257:G:N1    | 61:B2:1767:G:OP2   | 2.43                     | 0.52              |
| 62:A5:1895:U:H2'   | 62:A5:1896:A:C8    | 2.44                     | 0.52              |
| 73:AG:26:VAL:HG11  | 73:AG:40:ILE:HG21  | 1.92                     | 0.52              |
| 73:AG:43:ASP:O     | 73:AG:119:LYS:NZ   | 2.41                     | 0.52              |
| 77:CO:156:LYS:HA   | 77:CO:159:GLU:HB2  | 1.92                     | 0.52              |
| 2:CA:200:ARG:NH1   | 62:A5:2564:U:OP2   | 2.43                     | 0.52              |
| 7:Ag:150:ASP:OD2   | 16:AR:23:ARG:NH2   | 2.43                     | 0.52              |
| 12:AS:124:ARG:HH21 | 61:B2:1750:U:H5    | 1.57                     | 0.52              |
| 15:AL:35:ARG:NH2   | 15:AL:58:PRO:O     | 2.43                     | 0.52              |
| 25:Af:99:LYS:HE2   | 61:B2:1337:U:H3'   | 1.91                     | 0.52              |
| 26:AJ:89:ASP:OD1   | 26:AJ:92:ARG:NE    | 2.43                     | 0.52              |
| 27:Ca:83:VAL:HA    | 78:CL:164:VAL:HG11 | 1.92                     | 0.52              |
| 29:CI:187:ASP:OD1  | 29:CI:187:ASP:N    | 2.38                     | 0.52              |
| 33:CS:164:ARG:HH11 | 45:Cf:43:LYS:HD2   | 1.74                     | 0.52              |
| 46:CI:44:THR:HG23  | 46:CI:46:HIS:H     | 1.75                     | 0.52              |
| 46:CI:70:LEU:HA    | 46:CI:74:SER:HB2   | 1.92                     | 0.52              |
| 55:CE:101:LEU:N    | 55:CE:113:VAL:O    | 2.38                     | 0.52              |
| 55:CE:165:ASP:N    | 55:CE:165:ASP:OD1  | 2.43                     | 0.52              |
| 59:A8:77:G:H2'     | 59:A8:78:G:C8      | 2.45                     | 0.52              |
| 59:A8:101:A:OP1    | 83:Cj:21:ARG:NH2   | 2.43                     | 0.52              |
| 61:B2:1012:G:H2'   | 61:B2:1013:A:C8    | 2.45                     | 0.52              |
| 62:A5:1056:G:OP1   | 62:A5:2035:C:O2'   | 2.28                     | 0.52              |
| 62:A5:1359:G:N2    | 62:A5:1360:U:O2'   | 2.42                     | 0.52              |
| 62:A5:2882:A:OP2   | 62:A5:2884:C:N4    | 2.42                     | 0.52              |
| 69:AT:64:LEU:HD23  | 69:AT:69:PRO:HA    | 1.90                     | 0.52              |
| 72:AE:100:ARG:HG3  | 72:AE:114:ILE:HD13 | 1.92                     | 0.52              |
| 73:AG:133:LEU:HD11 | 73:AG:160:ARG:HD3  | 1.91                     | 0.52              |
| 2:CA:89:TYR:N      | 2:CA:100:ASN:OD1   | 2.43                     | 0.51              |
| 3:AB:164:VAL:O     | 3:AB:168:ARG:N     | 2.36                     | 0.51              |
| 6:CC:108:THR:O     | 6:CC:108:THR:OG1   | 2.25                     | 0.51              |
| 7:Ag:221:ASP:O     | 7:Ag:225:GLY:N     | 2.39                     | 0.51              |
| 12:AS:90:ILE:HG23  | 17:AP:21:ARG:HH21  | 1.75                     | 0.51              |
| 21:Aa:88:SER:HB3   | 21:Aa:91:ALA:H     | 1.74                     | 0.51              |
| 22:Ab:70:ARG:NH1   | 61:B2:1137:G:OP1   | 2.43                     | 0.51              |
| 27:Ca:56:LYS:NZ    | 62:A5:3319:A:OP1   | 2.41                     | 0.51              |
| 28:CN:105:ARG:NH2  | 62:A5:1788:G:OP2   | 2.42                     | 0.51              |
| 31:CQ:85:THR:HG22  | 31:CQ:104:HIS:HB3  | 1.91                     | 0.51              |
| 32:CR:103:ARG:HA   | 32:CR:106:LEU:HB2  | 1.92                     | 0.51              |
| 33:CS:75:ILE:HD12  | 33:CS:98:ARG:HH22  | 1.75                     | 0.51              |
| 34:CT:57:TYR:OH    | 62:A5:3256:U:OP1   | 2.24                     | 0.51              |
| 61:B2:92:A:H62     | 61:B2:401:G:H21    | 1.57                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 61:B2:92:A:O2'     | 72:AE:4:GLY:O      | 2.28                     | 0.51              |
| 61:B2:1804:U:OP1   | 70:AF:95:ARG:NH2   | 2.43                     | 0.51              |
| 62:A5:855:A:N6     | 62:A5:865:A:O5'    | 2.40                     | 0.51              |
| 62:A5:2572:G:O6    | 62:A5:2651:G:N2    | 2.43                     | 0.51              |
| 69:AT:70:ALA:O     | 69:AT:123:LEU:CD1  | 2.44                     | 0.51              |
| 7:Ag:19:THR:HA     | 7:Ag:288:LEU:HB3   | 1.92                     | 0.51              |
| 14:AN:39:LYS:O     | 14:AN:43:LYS:NZ    | 2.40                     | 0.51              |
| 18:AV:3:ASN:OD1    | 18:AV:7:GLU:N      | 2.41                     | 0.51              |
| 30:CD:41:LYS:NZ    | 34:CT:32:ARG:O     | 2.37                     | 0.51              |
| 32:CR:38:ARG:N     | 62:A5:1886:C:OP2   | 2.38                     | 0.51              |
| 35:CP:131:ARG:HH21 | 62:A5:1079:U:H1'   | 1.75                     | 0.51              |
| 40:Ch:88:THR:HG22  | 83:Cj:78:LEU:CD1   | 2.41                     | 0.51              |
| 54:CH:88:TYR:H     | 54:CH:144:VAL:HB   | 1.75                     | 0.51              |
| 62:A5:1345:G:N2    | 62:A5:2750:A:OP2   | 2.41                     | 0.51              |
| 62:A5:1742:U:H3    | 62:A5:1760:A:H61   | 1.58                     | 0.51              |
| 62:A5:2469:U:H3'   | 62:A5:2470:U:H2'   | 1.91                     | 0.51              |
| 66:Cg:15:THR:OG1   | 66:Cg:16:ARG:N     | 2.41                     | 0.51              |
| 72:AE:34:GLY:H     | 72:AE:83:PRO:HG2   | 1.75                     | 0.51              |
| 6:CC:50:ASN:ND2    | 62:A5:843:A:OP1    | 2.38                     | 0.51              |
| 11:AM:50:ASP:OD1   | 11:AM:50:ASP:N     | 2.43                     | 0.51              |
| 16:AR:16:ILE:HG22  | 23:AD:212:VAL:HG11 | 1.93                     | 0.51              |
| 28:CN:24:ARG:NH2   | 62:A5:2813:G:O2'   | 2.43                     | 0.51              |
| 35:CP:168:LYS:HD3  | 45:Cf:106:GLN:HB2  | 1.92                     | 0.51              |
| 55:CE:171:LEU:O    | 62:A5:3839:A:N6    | 2.44                     | 0.51              |
| 62:A5:862:U:O3'    | 78:CL:183:ARG:NH1  | 2.43                     | 0.51              |
| 62:A5:1083:A:O2'   | 62:A5:2518:A:N1    | 2.43                     | 0.51              |
| 64:AW:115:GLU:HG2  | 64:AW:118:ARG:HH21 | 1.75                     | 0.51              |
| 67:CU:272:LEU:HB3  | 67:CU:284:MET:HE2  | 1.92                     | 0.51              |
| 69:AT:29:LYS:CD    | 69:AT:105:GLN:C    | 2.80                     | 0.51              |
| 75:AI:64:ASN:HA    | 75:AI:75:LYS:HA    | 1.92                     | 0.51              |
| 2:CA:208:GLU:OE2   | 62:A5:1116:G:N2    | 2.44                     | 0.51              |
| 7:Ag:128:LYS:HG2   | 7:Ag:151:TRP:HA    | 1.93                     | 0.51              |
| 11:AM:132:LYS:HA   | 11:AM:135:LEU:HB2  | 1.92                     | 0.51              |
| 12:AS:117:ILE:HA   | 17:AP:114:MET:HE2  | 1.93                     | 0.51              |
| 20:AZ:79:ARG:HB3   | 20:AZ:83:ALA:HB2   | 1.92                     | 0.51              |
| 22:Ab:66:PRO:HA    | 61:B2:957:A:C6     | 2.46                     | 0.51              |
| 27:Ca:13:ARG:HH22  | 62:A5:811:G:P      | 2.32                     | 0.51              |
| 27:Ca:135:GLU:HA   | 27:Ca:138:ILE:HD12 | 1.91                     | 0.51              |
| 31:CQ:142:ARG:HB2  | 31:CQ:145:ALA:HB2  | 1.91                     | 0.51              |
| 31:CQ:164:ARG:H    | 62:A5:980:A:H5'    | 1.74                     | 0.51              |
| 32:CR:37:SER:HA    | 62:A5:1886:C:H5'   | 1.92                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 32:CR:96:MET:HG2   | 62:A5:2035:C:H5'   | 1.91                     | 0.51              |
| 32:CR:168:GLU:HA   | 32:CR:171:LYS:HB2  | 1.90                     | 0.51              |
| 45:Cf:53:LYS:HD2   | 45:Cf:147:ARG:HG2  | 1.93                     | 0.51              |
| 45:Cf:69:ASN:HA    | 45:Cf:138:ASN:HD21 | 1.74                     | 0.51              |
| 60:Cz:23:LYS:HE3   | 60:Cz:172:VAL:HG11 | 1.93                     | 0.51              |
| 61:B2:720:G:N1     | 61:B2:817:C:N3     | 2.57                     | 0.51              |
| 61:B2:1779:A:H2'   | 61:B2:1780:G:H8    | 1.76                     | 0.51              |
| 61:B2:1793:A:OP1   | 69:AT:91:HIS:CE1   | 2.64                     | 0.51              |
| 62:A5:122:C:O2     | 62:A5:159:G:N1     | 2.42                     | 0.51              |
| 64:AW:102:VAL:HG23 | 64:AW:128:PHE:HB3  | 1.92                     | 0.51              |
| 75:AI:106:ALA:HB2  | 75:AI:173:ILE:HG23 | 1.92                     | 0.51              |
| 1:AA:80:ARG:HG3    | 1:AA:129:THR:HG21  | 1.92                     | 0.51              |
| 6:CC:5:ASN:OD1     | 6:CC:5:ASN:N       | 2.44                     | 0.51              |
| 6:CC:7:ARG:NH1     | 6:CC:31:PHE:O      | 2.44                     | 0.51              |
| 6:CC:53:GLN:O      | 6:CC:114:TRP:NE1   | 2.43                     | 0.51              |
| 28:CN:68:ARG:NH2   | 62:A5:310:A:OP2    | 2.43                     | 0.51              |
| 33:CS:83:ARG:NH2   | 33:CS:92:ASN:OD1   | 2.35                     | 0.51              |
| 42:Cc:11:LEU:HB2   | 42:Cc:14:THR:HG23  | 1.92                     | 0.51              |
| 45:Cf:101:LYS:O    | 45:Cf:115:ARG:NH2  | 2.43                     | 0.51              |
| 61:B2:105:U:H5'    | 75:AI:21:LEU:HD21  | 1.92                     | 0.51              |
| 61:B2:494:C:H2'    | 61:B2:505:G:H22    | 1.76                     | 0.51              |
| 61:B2:1203:U:H2'   | 61:B2:1204:A:H8    | 1.76                     | 0.51              |
| 61:B2:1312:G:N1    | 61:B2:1345:U:O2'   | 2.44                     | 0.51              |
| 62:A5:1150:G:H21   | 62:A5:1610:A:H62   | 1.58                     | 0.51              |
| 62:A5:1372:A:H2'   | 62:A5:1373:A:H4'   | 1.92                     | 0.51              |
| 62:A5:3344:U:H2'   | 62:A5:3345:A:C8    | 2.45                     | 0.51              |
| 69:AT:23:LYS:CA    | 69:AT:28:LEU:CD2   | 2.88                     | 0.51              |
| 69:AT:129:ARG:CB   | 69:AT:133:ARG:CZ   | 2.72                     | 0.51              |
| 75:AI:48:THR:HG21  | 75:AI:54:LYS:H     | 1.76                     | 0.51              |
| 78:CL:116:LEU:HD23 | 78:CL:117:LYS:HG3  | 1.92                     | 0.51              |
| 81:B:6:A:H61       | 81:B:66:U:H3       | 1.57                     | 0.51              |
| 1:AA:6:ASP:N       | 1:AA:6:ASP:OD1     | 2.42                     | 0.51              |
| 2:CA:54:ARG:HE     | 2:CA:58:LEU:HD21   | 1.75                     | 0.51              |
| 2:CA:114:CYS:N     | 2:CA:165:MET:O     | 2.41                     | 0.51              |
| 3:AB:206:ARG:HH22  | 61:B2:1144:C:H1'   | 1.75                     | 0.51              |
| 5:AC:190:ALA:HB3   | 5:AC:193:PRO:HD3   | 1.93                     | 0.51              |
| 7:Ag:109:VAL:HA    | 7:Ag:125:SER:HB2   | 1.92                     | 0.51              |
| 12:AS:12:ILE:O     | 53:CJ:123:LYS:NZ   | 2.43                     | 0.51              |
| 24:Ae:87:GLN:O     | 61:B2:570:G:O2'    | 2.28                     | 0.51              |
| 27:Ca:145:CYS:SG   | 27:Ca:146:LEU:N    | 2.83                     | 0.51              |
| 28:CN:5:ARG:NH1    | 62:A5:283:A:O2'    | 2.44                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 31:CQ:92:LEU:O    | 31:CQ:112:ARG:NH2 | 2.39                     | 0.51              |
| 34:CT:66:ASN:HB2  | 34:CT:73:GLY:H    | 1.76                     | 0.51              |
| 40:Ch:70:ARG:NH1  | 62:A5:139:U:O4    | 2.44                     | 0.51              |
| 61:B2:211:U:O2    | 61:B2:259:G:N2    | 2.39                     | 0.51              |
| 61:B2:831:U:H3    | 61:B2:885:U:H3    | 1.58                     | 0.51              |
| 62:A5:704:U:O4    | 62:A5:733:A:N6    | 2.42                     | 0.51              |
| 62:A5:1163:G:N2   | 62:A5:1164:G:N3   | 2.59                     | 0.51              |
| 62:A5:1221:U:H2'  | 62:A5:1222:A:H8   | 1.76                     | 0.51              |
| 62:A5:1540:U:O4   | 62:A5:1541:A:N6   | 2.43                     | 0.51              |
| 62:A5:1804:A:N6   | 62:A5:1862:U:O4   | 2.43                     | 0.51              |
| 62:A5:2061:G:H3'  | 62:A5:2062:A:C8   | 2.45                     | 0.51              |
| 62:A5:2268:G:O2'  | 62:A5:2474:A:N1   | 2.41                     | 0.51              |
| 69:AT:50:PRO:CD   | 69:AT:51:ASP:N    | 2.73                     | 0.51              |
| 2:CA:205:ASN:O    | 2:CA:207:VAL:N    | 2.43                     | 0.51              |
| 4:CB:102:LEU:HG   | 4:CB:103:VAL:HG23 | 1.93                     | 0.51              |
| 9:AO:45:THR:OG1   | 9:AO:46:ASP:N     | 2.43                     | 0.51              |
| 14:AN:69:ASN:HA   | 14:AN:73:ARG:HH21 | 1.75                     | 0.51              |
| 29:CI:215:ASP:N   | 29:CI:215:ASP:OD1 | 2.42                     | 0.51              |
| 30:CD:234:ASP:OD1 | 30:CD:234:ASP:N   | 2.42                     | 0.51              |
| 33:CS:97:TYR:OH   | 33:CS:112:ASP:OD2 | 2.21                     | 0.51              |
| 53:CJ:57:LYS:HA   | 53:CJ:72:LYS:H    | 1.75                     | 0.51              |
| 53:CJ:78:THR:OG1  | 58:A7:39:C:N3     | 2.42                     | 0.51              |
| 54:CH:9:CYS:SG    | 54:CH:52:THR:OG1  | 2.67                     | 0.51              |
| 61:B2:1328:G:N2   | 61:B2:1644:U:O2   | 2.44                     | 0.51              |
| 61:B2:1777:U:H4'  | 76:AQ:140:ARG:HD3 | 1.93                     | 0.51              |
| 61:B2:1882:C:O2   | 61:B2:1904:G:N1   | 2.43                     | 0.51              |
| 62:A5:3017:U:O2'  | 62:A5:3101:A:N1   | 2.43                     | 0.51              |
| 62:A5:3098:A:OP1  | 62:A5:3101:A:N6   | 2.44                     | 0.51              |
| 62:A5:3477:A:H5'' | 62:A5:3478:G:H5'  | 1.91                     | 0.51              |
| 76:AQ:132:LYS:HA  | 76:AQ:139:ALA:HA  | 1.90                     | 0.51              |
| 14:AN:142:GLU:O   | 14:AN:145:THR:OG1 | 2.28                     | 0.51              |
| 16:AR:5:ARG:H     | 61:B2:1594:A:H62  | 1.59                     | 0.51              |
| 40:Ch:89:ARG:HH22 | 59:A8:36:A:H2     | 1.59                     | 0.51              |
| 55:CE:40:LYS:HB2  | 55:CE:42:ARG:HD3  | 1.92                     | 0.51              |
| 61:B2:941:A:HO2'  | 61:B2:943:U:HO2'  | 1.51                     | 0.51              |
| 61:B2:1444:C:C2'  | 69:AT:129:ARG:NE  | 2.74                     | 0.51              |
| 61:B2:1583:A:O2'  | 61:B2:1585:A:OP2  | 2.25                     | 0.51              |
| 62:A5:584:A:O2'   | 62:A5:628:A:N1    | 2.39                     | 0.51              |
| 62:A5:2746:A:H2'  | 62:A5:2747:G:H8   | 1.74                     | 0.51              |
| 4:CB:119:TYR:OH   | 4:CB:129:ALA:N    | 2.42                     | 0.51              |
| 5:AC:60:SER:OG    | 5:AC:62:GLU:OE1   | 2.28                     | 0.51              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 6:CC:5:ASN:HD21   | 62:A5:497:U:H5''   | 1.75                     | 0.51              |
| 12:AS:124:ARG:NH2 | 17:AP:126:TYR:OH   | 2.44                     | 0.51              |
| 21:Aa:2:THR:N     | 61:B2:1230:A:OP1   | 2.44                     | 0.51              |
| 27:Ca:114:GLY:N   | 62:A5:865:A:OP2    | 2.39                     | 0.51              |
| 28:CN:144:ARG:NH2 | 62:A5:130:C:OP1    | 2.44                     | 0.51              |
| 55:CE:48:LYS:NZ   | 62:A5:681:G:O5'    | 2.42                     | 0.51              |
| 59:A8:28:A:H5''   | 78:CL:26:ASN:HB3   | 1.92                     | 0.51              |
| 60:Cz:135:PRO:HA  | 60:Cz:156:LYS:HE3  | 1.92                     | 0.51              |
| 61:B2:421:A:H3'   | 61:B2:422:A:H8     | 1.76                     | 0.51              |
| 62:A5:2061:G:H5'' | 62:A5:2062:A:H2'   | 1.93                     | 0.51              |
| 62:A5:2161:G:H4'  | 83:Cj:8:PHE:CD2    | 2.46                     | 0.51              |
| 62:A5:3718:A:H1'  | 77:CO:117:ARG:HD2  | 1.92                     | 0.51              |
| 64:AW:74:VAL:HA   | 64:AW:127:GLY:HA2  | 1.93                     | 0.51              |
| 69:AT:23:LYS:HG2  | 69:AT:28:LEU:HD22  | 1.89                     | 0.51              |
| 75:AI:24:LYS:O    | 75:AI:25:ARG:NH1   | 2.44                     | 0.51              |
| 78:CL:178:ALA:O   | 78:CL:181:THR:OG1  | 2.29                     | 0.51              |
| 81:B:29:G:H1      | 81:B:39:U:H3       | 1.57                     | 0.51              |
| 83:Cj:72:ARG:HB3  | 83:Cj:72:ARG:NH2   | 2.26                     | 0.51              |
| 5:AC:248:PRO:HA   | 5:AC:251:ALA:HB3   | 1.93                     | 0.51              |
| 6:CC:336:GLU:OE2  | 6:CC:340:ARG:NH2   | 2.44                     | 0.51              |
| 9:AO:45:THR:HA    | 9:AO:52:THR:HA     | 1.92                     | 0.51              |
| 23:AD:119:ARG:HE  | 24:Ae:123:ARG:HH21 | 1.57                     | 0.51              |
| 28:CN:68:ARG:HE   | 62:A5:309:C:P      | 2.33                     | 0.51              |
| 28:CN:178:TYR:O   | 28:CN:179:ARG:NE   | 2.44                     | 0.51              |
| 31:CQ:89:ASP:OD2  | 31:CQ:91:ARG:NH2   | 2.44                     | 0.51              |
| 38:CZ:54:THR:HG23 | 38:CZ:56:LYS:H     | 1.75                     | 0.51              |
| 61:B2:90:A:OP1    | 61:B2:402:A:N6     | 2.45                     | 0.51              |
| 61:B2:332:U:H2'   | 61:B2:333:A:C8     | 2.46                     | 0.51              |
| 61:B2:1552:C:O2   | 61:B2:1559:A:N6    | 2.44                     | 0.51              |
| 61:B2:1778:A:H5'' | 76:AQ:141:ALA:HB2  | 1.92                     | 0.51              |
| 62:A5:660:A:H2'   | 62:A5:661:G:H8     | 1.76                     | 0.51              |
| 62:A5:1023:C:O2'  | 62:A5:1778:A:O2'   | 2.26                     | 0.51              |
| 62:A5:1398:C:O3'  | 80:CM:51:ARG:NH2   | 2.44                     | 0.51              |
| 70:AF:99:SER:OG   | 70:AF:179:CYS:SG   | 2.68                     | 0.51              |
| 71:CF:144:THR:O   | 71:CF:144:THR:OG1  | 2.19                     | 0.51              |
| 74:AH:104:ARG:HB2 | 74:AH:107:ARG:HB2  | 1.92                     | 0.51              |
| 80:CM:11:ARG:HE   | 80:CM:61:ARG:HB2   | 1.76                     | 0.51              |
| 2:CA:226:LYS:NZ   | 62:A5:3136:U:O2'   | 2.43                     | 0.50              |
| 7:Ag:155:VAL:O    | 7:Ag:156:ARG:NH1   | 2.39                     | 0.50              |
| 14:AN:121:ARG:NH1 | 61:B2:954:A:OP1    | 2.36                     | 0.50              |
| 22:Ab:56:CYS:SG   | 22:Ab:57:ALA:N     | 2.84                     | 0.50              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 40:Ch:66:LYS:HE3  | 59:A8:94:C:H5'     | 1.93                     | 0.50              |
| 41:Cb:43:GLN:O    | 41:Cb:47:ARG:N     | 2.38                     | 0.50              |
| 55:CE:57:LYS:HA   | 55:CE:64:LYS:HG3   | 1.93                     | 0.50              |
| 61:B2:1249:C:O2'  | 63:Ac:20:GLN:NE2   | 2.36                     | 0.50              |
| 61:B2:1452:U:N3   | 61:B2:1453:G:O6    | 2.44                     | 0.50              |
| 61:B2:1457:C:O2   | 61:B2:1459:G:N2    | 2.44                     | 0.50              |
| 61:B2:1757:G:OP1  | 69:AT:38:LYS:HE3   | 2.11                     | 0.50              |
| 61:B2:1773:C:OP1  | 76:AQ:142:ARG:NH1  | 2.40                     | 0.50              |
| 62:A5:2082:U:H2'  | 62:A5:2083:G:H8    | 1.76                     | 0.50              |
| 67:CU:264:LYS:HD3 | 67:CU:267:SER:HA   | 1.92                     | 0.50              |
| 71:CF:190:CYS:SG  | 71:CF:191:VAL:N    | 2.84                     | 0.50              |
| 78:CL:120:ARG:O   | 78:CL:120:ARG:NH2  | 2.43                     | 0.50              |
| 80:CM:7:VAL:HG22  | 80:CM:57:LEU:HD22  | 1.93                     | 0.50              |
| 5:AC:222:ALA:O    | 5:AC:226:ALA:N     | 2.44                     | 0.50              |
| 18:AV:34:MET:SD   | 18:AV:35:ASN:N     | 2.84                     | 0.50              |
| 21:Aa:60:ASP:OD1  | 21:Aa:60:ASP:N     | 2.42                     | 0.50              |
| 23:AD:173:ALA:HB3 | 23:AD:188:VAL:HG22 | 1.92                     | 0.50              |
| 24:Ae:95:GLU:HB3  | 24:Ae:96:LYS:HD3   | 1.93                     | 0.50              |
| 28:CN:181:SER:OG  | 62:A5:299:G:O6     | 2.28                     | 0.50              |
| 31:CQ:81:VAL:HG22 | 31:CQ:101:CYS:HB3  | 1.93                     | 0.50              |
| 46:Ci:94:LYS:NZ   | 62:A5:327:C:OP1    | 2.34                     | 0.50              |
| 53:CJ:116:GLU:HA  | 53:CJ:130:ILE:HD11 | 1.93                     | 0.50              |
| 55:CE:174:LYS:NZ  | 55:CE:190:GLU:OE2  | 2.38                     | 0.50              |
| 59:A8:108:A:C8    | 83:Cj:29:LEU:HD21  | 2.46                     | 0.50              |
| 60:Cz:160:LYS:HD2 | 60:Cz:164:CYS:HB3  | 1.93                     | 0.50              |
| 61:B2:1822:U:O2'  | 61:B2:1959:C:O2'   | 2.27                     | 0.50              |
| 62:A5:1907:U:H2'  | 62:A5:2134:A:H61   | 1.76                     | 0.50              |
| 62:A5:2502:G:H2'  | 62:A5:2503:G:H8    | 1.76                     | 0.50              |
| 62:A5:3153:G:N1   | 81:B:72:A:O2'      | 2.43                     | 0.50              |
| 69:AT:10:ASP:OD1  | 76:AQ:43:GLN:O     | 2.30                     | 0.50              |
| 72:AE:92:LEU:HB3  | 72:AE:97:GLU:HB2   | 1.91                     | 0.50              |
| 1:AA:206:ASP:N    | 1:AA:206:ASP:OD1   | 2.44                     | 0.50              |
| 6:CC:185:LYS:NZ   | 62:A5:1627:U:O2    | 2.39                     | 0.50              |
| 8:AU:31:VAL:O     | 8:AU:35:GLU:N      | 2.44                     | 0.50              |
| 9:AO:135:ILE:O    | 61:B2:973:U:O2'    | 2.29                     | 0.50              |
| 12:AS:124:ARG:HG2 | 12:AS:129:LEU:HD13 | 1.94                     | 0.50              |
| 14:AN:140:LYS:NZ  | 62:A5:1045:G:O6    | 2.40                     | 0.50              |
| 17:AP:57:MET:O    | 17:AP:61:LYS:N     | 2.42                     | 0.50              |
| 28:CN:23:LEU:HD11 | 28:CN:122:ALA:HB2  | 1.94                     | 0.50              |
| 29:CI:153:ARG:NH2 | 62:A5:1507:C:OP1   | 2.43                     | 0.50              |
| 29:CI:210:GLU:OE2 | 29:CI:214:ARG:NE   | 2.44                     | 0.50              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 33:CS:176:PHE:O   | 62:A5:3752:G:O2'   | 2.27                     | 0.50              |
| 56:CG:38:GLU:HG2  | 56:CG:40:ARG:HH11  | 1.75                     | 0.50              |
| 56:CG:195:LEU:HB3 | 56:CG:207:LEU:HD23 | 1.93                     | 0.50              |
| 62:A5:829:U:O2'   | 62:A5:988:C:O2     | 2.28                     | 0.50              |
| 62:A5:1323:C:H5'' | 62:A5:1324:C:H5''  | 1.93                     | 0.50              |
| 62:A5:3308:A:H5'' | 62:A5:3309:A:H5'   | 1.92                     | 0.50              |
| 64:AW:37:PHE:HD1  | 64:AW:110:ILE:HD11 | 1.76                     | 0.50              |
| 70:AF:209:SER:O   | 70:AF:215:LYS:NZ   | 2.39                     | 0.50              |
| 72:AE:212:ASP:OD1 | 72:AE:216:HIS:N    | 2.40                     | 0.50              |
| 78:CL:147:THR:HB  | 78:CL:149:LEU:HG   | 1.93                     | 0.50              |
| 1:AA:7:ILE:HA     | 1:AA:11:LYS:HD3    | 1.92                     | 0.50              |
| 2:CA:117:GLU:O    | 2:CA:162:ASN:ND2   | 2.45                     | 0.50              |
| 2:CA:203:ALA:O    | 62:A5:1114:A:O2'   | 2.29                     | 0.50              |
| 3:AB:124:ILE:O    | 3:AB:144:GLY:N     | 2.41                     | 0.50              |
| 4:CB:294:LYS:HD3  | 4:CB:298:VAL:HG21  | 1.94                     | 0.50              |
| 6:CC:85:GLY:HA2   | 6:CC:87:THR:HG22   | 1.93                     | 0.50              |
| 9:AO:31:ALA:HA    | 9:AO:44:VAL:HG22   | 1.92                     | 0.50              |
| 17:AP:37:VAL:HA   | 17:AP:40:MET:HB2   | 1.92                     | 0.50              |
| 17:AP:111:LYS:HB2 | 17:AP:114:MET:HE3  | 1.93                     | 0.50              |
| 32:CR:81:ARG:NE   | 62:A5:2482:C:OP1   | 2.41                     | 0.50              |
| 45:Cf:8:SER:HA    | 45:Cf:22:LYS:HG2   | 1.92                     | 0.50              |
| 47:Ck:40:ARG:NH2  | 62:A5:1898:C:OP1   | 2.45                     | 0.50              |
| 59:A8:82:C:H3'    | 59:A8:83:A:H2'     | 1.94                     | 0.50              |
| 60:Cz:17:LEU:O    | 60:Cz:176:SER:OG   | 2.29                     | 0.50              |
| 61:B2:378:G:N2    | 61:B2:611:U:O2'    | 2.42                     | 0.50              |
| 61:B2:1079:A:O2'  | 61:B2:1980:U:O2    | 2.29                     | 0.50              |
| 61:B2:1136:U:H2'  | 61:B2:1137:G:H8    | 1.76                     | 0.50              |
| 62:A5:211:U:H3'   | 62:A5:212:U:H4'    | 1.92                     | 0.50              |
| 62:A5:268:U:H2'   | 62:A5:269:A:H8     | 1.76                     | 0.50              |
| 62:A5:817:C:H2'   | 62:A5:818:A:H8     | 1.77                     | 0.50              |
| 62:A5:1504:C:H2'  | 62:A5:1505:A:H8    | 1.76                     | 0.50              |
| 69:AT:30:VAL:HG12 | 69:AT:31:PRO:HD2   | 1.94                     | 0.50              |
| 3:AB:199:ASP:N    | 3:AB:199:ASP:OD1   | 2.44                     | 0.50              |
| 5:AC:96:GLN:N     | 61:B2:11:A:O2'     | 2.41                     | 0.50              |
| 6:CC:385:LEU:HA   | 6:CC:388:ARG:HG2   | 1.93                     | 0.50              |
| 10:AX:49:GLY:N    | 10:AX:100:VAL:O    | 2.41                     | 0.50              |
| 17:AP:95:SER:OG   | 17:AP:96:ILE:N     | 2.45                     | 0.50              |
| 23:AD:41:VAL:HG13 | 23:AD:50:ILE:HG13  | 1.93                     | 0.50              |
| 29:CI:97:ILE:HG13 | 29:CI:99:ILE:HD11  | 1.94                     | 0.50              |
| 32:CR:112:SER:OG  | 32:CR:113:LYS:N    | 2.45                     | 0.50              |
| 32:CR:125:MET:O   | 32:CR:129:GLY:N    | 2.45                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 33:CS:55:LYS:NZ    | 58:A7:75:G:O6      | 2.34                     | 0.50              |
| 34:CT:141:VAL:N    | 71:CF:84:PHE:O     | 2.42                     | 0.50              |
| 35:CP:3:ARG:HE     | 62:A5:416:C:H5''   | 1.77                     | 0.50              |
| 37:CY:115:ARG:HH21 | 59:A8:70:A:H5''    | 1.76                     | 0.50              |
| 47:Ck:52:LYS:HG2   | 47:Ck:55:LYS:HD2   | 1.93                     | 0.50              |
| 51:Cp:4:ARG:NH2    | 62:A5:1039:U:O4    | 2.44                     | 0.50              |
| 54:CH:47:MET:HA    | 54:CH:53:LEU:HA    | 1.92                     | 0.50              |
| 60:Cz:32:VAL:HG12  | 60:Cz:170:GLY:H    | 1.76                     | 0.50              |
| 61:B2:355:G:O2'    | 61:B2:1057:A:N1    | 2.44                     | 0.50              |
| 61:B2:886:G:H21    | 64:AW:121:LEU:HD11 | 1.75                     | 0.50              |
| 61:B2:1671:U:N3    | 69:AT:82:ARG:CZ    | 2.74                     | 0.50              |
| 62:A5:1280:C:H42   | 62:A5:1305:A:H61   | 1.59                     | 0.50              |
| 62:A5:3909:A:OP2   | 62:A5:3942:U:N3    | 2.41                     | 0.50              |
| 68:AK:15:LEU:HD13  | 68:AK:21:ILE:HB    | 1.94                     | 0.50              |
| 69:AT:135:ALA:HA   | 69:AT:138:ILE:HD12 | 1.93                     | 0.50              |
| 70:AF:54:VAL:O     | 70:AF:60:GLN:NE2   | 2.41                     | 0.50              |
| 72:AE:198:ARG:HH12 | 72:AE:200:ARG:HH11 | 1.60                     | 0.50              |
| 74:AH:41:ASP:OD1   | 74:AH:43:HIS:NE2   | 2.45                     | 0.50              |
| 74:AH:163:THR:HG23 | 74:AH:164:ILE:HG23 | 1.93                     | 0.50              |
| 75:AI:39:GLY:N     | 75:AI:60:LEU:O     | 2.40                     | 0.50              |
| 1:AA:71:PRO:HB2    | 1:AA:95:ASP:HB2    | 1.92                     | 0.50              |
| 2:CA:223:SER:O     | 2:CA:223:SER:OG    | 2.20                     | 0.50              |
| 6:CC:42:GLU:HA     | 6:CC:45:GLN:HE21   | 1.77                     | 0.50              |
| 7:Ag:221:ASP:N     | 7:Ag:221:ASP:OD1   | 2.44                     | 0.50              |
| 21:Aa:23:CYS:SG    | 21:Aa:24:THR:N     | 2.84                     | 0.50              |
| 24:Ae:105:LYS:NZ   | 61:B2:601:U:O4     | 2.40                     | 0.50              |
| 30:CD:15:ARG:NH1   | 62:A5:3221:A:OP2   | 2.44                     | 0.50              |
| 36:CX:169:ARG:NH2  | 62:A5:1805:A:OP2   | 2.44                     | 0.50              |
| 39:Cr:25:VAL:HB    | 39:Cr:28:PRO:HG3   | 1.92                     | 0.50              |
| 40:Ch:9:LEU:HA     | 40:Ch:12:LYS:HD3   | 1.94                     | 0.50              |
| 60:Cz:105:LYS:HD2  | 60:Cz:131:ALA:HB2  | 1.94                     | 0.50              |
| 61:B2:109:U:O2'    | 61:B2:882:G:N2     | 2.44                     | 0.50              |
| 61:B2:1686:C:H42   | 61:B2:1705:G:H1    | 1.58                     | 0.50              |
| 61:B2:1777:U:H2'   | 61:B2:1778:A:H8    | 1.77                     | 0.50              |
| 62:A5:702:A:C5     | 62:A5:703:A:H1'    | 2.46                     | 0.50              |
| 62:A5:1405:U:H1'   | 77:CO:50:TYR:HE2   | 1.76                     | 0.50              |
| 62:A5:1983:A:H61   | 62:A5:2089:A:H61   | 1.59                     | 0.50              |
| 62:A5:2543:C:N4    | 62:A5:2548:G:O6    | 2.45                     | 0.50              |
| 62:A5:2771:G:H22   | 62:A5:3516:C:N4    | 2.09                     | 0.50              |
| 62:A5:3265:C:H2'   | 62:A5:3266:A:H8    | 1.76                     | 0.50              |
| 69:AT:10:ASP:OD1   | 76:AQ:44:ILE:HA    | 2.11                     | 0.50              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 75:AI:66:ALA:HA   | 75:AI:73:ALA:HA    | 1.93                     | 0.50              |
| 77:CO:12:ASP:OD2  | 77:CO:39:ARG:NH1   | 2.44                     | 0.50              |
| 2:CA:208:GLU:OE1  | 62:A5:1112:G:N1    | 2.36                     | 0.50              |
| 4:CB:182:GLU:OE2  | 62:A5:3537:U:O2'   | 2.29                     | 0.50              |
| 4:CB:274:TYR:HE1  | 4:CB:343:ARG:HH22  | 1.60                     | 0.50              |
| 5:AC:212:SER:O    | 5:AC:215:THR:OG1   | 2.26                     | 0.50              |
| 6:CC:193:ARG:NH2  | 62:A5:1623:G:OP2   | 2.44                     | 0.50              |
| 9:AO:52:THR:HG21  | 61:B2:982:G:H21    | 1.77                     | 0.50              |
| 12:AS:88:LYS:HG2  | 17:AP:21:ARG:HD2   | 1.94                     | 0.50              |
| 14:AN:93:LYS:HB2  | 14:AN:150:VAL:HG21 | 1.94                     | 0.50              |
| 29:CI:149:ILE:HA  | 29:CI:152:LEU:HB2  | 1.94                     | 0.50              |
| 30:CD:144:CYS:N   | 30:CD:172:ASN:O    | 2.44                     | 0.50              |
| 34:CT:14:MET:HB3  | 34:CT:15:PHE:HD1   | 1.76                     | 0.50              |
| 37:CY:8:SER:HB2   | 62:A5:353:G:H5'    | 1.92                     | 0.50              |
| 38:CZ:26:VAL:HG12 | 38:CZ:93:GLU:HB3   | 1.94                     | 0.50              |
| 38:CZ:102:ASP:OD1 | 38:CZ:102:ASP:N    | 2.45                     | 0.50              |
| 56:CG:145:THR:OG1 | 62:A5:155:U:OP2    | 2.25                     | 0.50              |
| 61:B2:473:A:N1    | 61:B2:602:A:O2'    | 2.37                     | 0.50              |
| 61:B2:1968:C:H2'  | 61:B2:1969:G:C8    | 2.47                     | 0.50              |
| 62:A5:108:A:H2'   | 62:A5:109:A:C8     | 2.46                     | 0.50              |
| 62:A5:2496:A:N6   | 62:A5:2497:C:N3    | 2.59                     | 0.50              |
| 62:A5:2829:G:N1   | 62:A5:2889:C:O2    | 2.44                     | 0.50              |
| 62:A5:3592:C:O4'  | 62:A5:3621:A:N6    | 2.44                     | 0.50              |
| 65:CW:34:LYS:HG2  | 65:CW:38:ARG:HG2   | 1.92                     | 0.50              |
| 66:Cg:71:THR:OG1  | 66:Cg:72:VAL:N     | 2.43                     | 0.50              |
| 68:AK:2:PHE:O     | 68:AK:8:ARG:NH2    | 2.40                     | 0.50              |
| 71:CF:220:PRO:HD3 | 71:CF:251:MET:HG3  | 1.94                     | 0.50              |
| 3:AB:35:ALA:HB2   | 3:AB:44:ILE:HD11   | 1.94                     | 0.50              |
| 4:CB:128:LYS:NZ   | 62:A5:3685:U:OP1   | 2.45                     | 0.50              |
| 8:AU:78:THR:OG1   | 8:AU:79:TRP:N      | 2.39                     | 0.50              |
| 33:CS:95:ARG:NH2  | 33:CS:112:ASP:OD2  | 2.45                     | 0.50              |
| 41:Cb:38:LYS:HZ1  | 41:Cb:45:TYR:HE2   | 1.60                     | 0.50              |
| 44:Ce:11:ILE:HD11 | 44:Ce:68:MET:HE2   | 1.93                     | 0.50              |
| 61:B2:222:C:O2'   | 61:B2:922:G:N2     | 2.45                     | 0.50              |
| 61:B2:368:G:H2'   | 61:B2:369:G:H8     | 1.77                     | 0.50              |
| 61:B2:444:U:O4'   | 61:B2:470:G:N2     | 2.45                     | 0.50              |
| 61:B2:492:G:H21   | 61:B2:508:C:H41    | 1.58                     | 0.50              |
| 61:B2:1018:C:H5'' | 61:B2:1019:U:H5''  | 1.94                     | 0.50              |
| 62:A5:652:G:N2    | 62:A5:655:C:O5'    | 2.45                     | 0.50              |
| 62:A5:671:A:N7    | 62:A5:673:U:O2'    | 2.40                     | 0.50              |
| 62:A5:700:A:H61   | 62:A5:736:A:H61    | 1.60                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 62:A5:763:A:N6     | 62:A5:767:A:O2'    | 2.44                     | 0.50              |
| 62:A5:1341:G:H21   | 62:A5:1343:A:H8    | 1.60                     | 0.50              |
| 62:A5:1560:A:H2'   | 62:A5:1561:G:C8    | 2.45                     | 0.50              |
| 62:A5:1985:C:O2    | 62:A5:2088:G:N1    | 2.45                     | 0.50              |
| 73:AG:172:SER:OG   | 73:AG:173:LYS:N    | 2.45                     | 0.50              |
| 77:CO:13:GLY:HA2   | 77:CO:16:HIS:HB2   | 1.93                     | 0.50              |
| 4:CB:311:ASP:OD1   | 4:CB:311:ASP:N     | 2.44                     | 0.50              |
| 14:AN:69:ASN:OD1   | 61:B2:945:A:N7     | 2.45                     | 0.50              |
| 17:AP:98:GLY:HA2   | 17:AP:107:GLN:HA   | 1.94                     | 0.50              |
| 23:AD:111:LEU:HD21 | 23:AD:177:VAL:HG11 | 1.94                     | 0.50              |
| 28:CN:113:LEU:HB2  | 28:CN:134:LEU:HD22 | 1.93                     | 0.50              |
| 33:CS:140:VAL:HG22 | 54:CH:1:MET:HE1    | 1.93                     | 0.50              |
| 41:Cb:71:PRO:HG2   | 41:Cb:72:LYS:HD3   | 1.93                     | 0.50              |
| 61:B2:292:G:H4'    | 61:B2:293:A:H5'    | 1.94                     | 0.50              |
| 61:B2:1984:G:H2'   | 61:B2:1985:A:C8    | 2.46                     | 0.50              |
| 62:A5:358:C:O2'    | 62:A5:362:A:N3     | 2.44                     | 0.50              |
| 62:A5:1020:A:N3    | 62:A5:1111:C:O2'   | 2.45                     | 0.50              |
| 62:A5:1994:U:O2    | 67:CU:261:ARG:NH1  | 2.45                     | 0.50              |
| 78:CL:126:PHE:HE1  | 78:CL:142:GLU:HA   | 1.77                     | 0.50              |
| 1:AA:180:ARG:O     | 1:AA:184:ARG:N     | 2.40                     | 0.49              |
| 2:CA:80:GLU:OE2    | 2:CA:81:GLY:N      | 2.45                     | 0.49              |
| 10:AX:6:GLY:N      | 61:B2:1191:C:OP1   | 2.45                     | 0.49              |
| 19:AY:111:ARG:HA   | 19:AY:114:ARG:HD2  | 1.94                     | 0.49              |
| 23:AD:11:ARG:NH1   | 61:B2:1682:A:OP2   | 2.45                     | 0.49              |
| 26:AJ:82:LEU:HD13  | 26:AJ:85:ILE:HD11  | 1.93                     | 0.49              |
| 30:CD:273:LEU:O    | 30:CD:278:ARG:NH1  | 2.45                     | 0.49              |
| 36:CX:210:LYS:O    | 36:CX:216:THR:OG1  | 2.28                     | 0.49              |
| 38:CZ:55:LYS:NZ    | 62:A5:3008:U:OP2   | 2.41                     | 0.49              |
| 44:Ce:61:SER:N     | 62:A5:1646:U:OP1   | 2.40                     | 0.49              |
| 45:Cf:76:GLU:OE2   | 77:CO:5:THR:OG1    | 2.30                     | 0.49              |
| 47:Ck:37:ARG:NH2   | 47:Ck:41:PHE:O     | 2.43                     | 0.49              |
| 52:Co:43:ARG:HD2   | 62:A5:303:G:N2     | 2.27                     | 0.49              |
| 52:Co:99:GLY:O     | 53:CJ:57:LYS:NZ    | 2.37                     | 0.49              |
| 53:CJ:22:ILE:HA    | 53:CJ:139:LEU:HA   | 1.93                     | 0.49              |
| 60:Cz:101:LYS:NZ   | 62:A5:2872:U:O4    | 2.44                     | 0.49              |
| 61:B2:66:C:N4      | 73:AG:134:GLY:O    | 2.44                     | 0.49              |
| 61:B2:252:A:O2'    | 61:B2:254:C:OP2    | 2.29                     | 0.49              |
| 61:B2:913:G:H1     | 61:B2:928:C:H42    | 1.59                     | 0.49              |
| 61:B2:1089:G:N2    | 61:B2:1955:G:O3'   | 2.36                     | 0.49              |
| 62:A5:1153:G:OP1   | 62:A5:1168:G:N2    | 2.40                     | 0.49              |
| 69:AT:11:GLN:HG2   | 69:AT:14:VAL:HB    | 1.93                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 69:AT:129:ARG:HG2  | 69:AT:133:ARG:HE   | 1.76                     | 0.49              |
| 2:CA:84:THR:HG22   | 51:Cp:63:THR:H     | 1.76                     | 0.49              |
| 3:AB:75:GLN:O      | 3:AB:82:ARG:NH2    | 2.41                     | 0.49              |
| 3:AB:88:ARG:N      | 3:AB:105:GLY:O     | 2.46                     | 0.49              |
| 4:CB:26:ARG:NE     | 62:A5:3537:U:OP1   | 2.45                     | 0.49              |
| 6:CC:112:ARG:HB2   | 6:CC:114:TRP:HE3   | 1.77                     | 0.49              |
| 15:AL:32:ARG:NH1   | 15:AL:50:GLY:O     | 2.45                     | 0.49              |
| 16:AR:92:GLU:H     | 16:AR:95:ILE:HG22  | 1.77                     | 0.49              |
| 19:AY:11:ARG:NH2   | 61:B2:862:C:O2'    | 2.46                     | 0.49              |
| 30:CD:179:ARG:NH2  | 62:A5:3278:A:OP2   | 2.46                     | 0.49              |
| 33:CS:132:ILE:HD12 | 33:CS:133:PRO:HD2  | 1.95                     | 0.49              |
| 33:CS:170:ARG:HH11 | 62:A5:3721:C:H42   | 1.59                     | 0.49              |
| 55:CE:34:SER:HA    | 55:CE:37:GLN:HE22  | 1.77                     | 0.49              |
| 56:CG:205:THR:HG23 | 56:CG:206:THR:HG23 | 1.93                     | 0.49              |
| 62:A5:795:A:O4'    | 62:A5:2750:A:N6    | 2.45                     | 0.49              |
| 62:A5:3228:A:H61   | 62:A5:3289:U:H3    | 1.60                     | 0.49              |
| 64:AW:51:GLU:OE2   | 74:AH:143:ARG:NH2  | 2.42                     | 0.49              |
| 71:CF:169:ARG:HE   | 71:CF:213:TRP:CD1  | 2.30                     | 0.49              |
| 74:AH:145:LYS:HE3  | 74:AH:151:LEU:HB2  | 1.93                     | 0.49              |
| 76:AQ:1:MET:O      | 76:AQ:2:GLN:NE2    | 2.40                     | 0.49              |
| 2:CA:35:ALA:O      | 2:CA:39:GLY:N      | 2.44                     | 0.49              |
| 7:Ag:69:ASP:HB3    | 7:Ag:111:SER:HA    | 1.94                     | 0.49              |
| 12:AS:115:LYS:O    | 12:AS:118:ARG:NH1  | 2.45                     | 0.49              |
| 24:Ae:125:ARG:HH22 | 24:Ae:127:PRO:HA   | 1.77                     | 0.49              |
| 26:AJ:64:LEU:O     | 26:AJ:71:ARG:NH1   | 2.45                     | 0.49              |
| 26:AJ:176:ARG:HH21 | 26:AJ:179:LEU:HD11 | 1.77                     | 0.49              |
| 27:Ca:94:GLU:OE2   | 27:Ca:121:ARG:NH2  | 2.45                     | 0.49              |
| 35:CP:42:ARG:NH1   | 35:CP:99:GLU:OE2   | 2.45                     | 0.49              |
| 39:Cr:50:LYS:HB3   | 39:Cr:72:LYS:HD2   | 1.94                     | 0.49              |
| 42:Cc:51:ASN:ND2   | 42:Cc:51:ASN:N     | 2.32                     | 0.49              |
| 59:A8:75:C:H2'     | 59:A8:76:A:C8      | 2.47                     | 0.49              |
| 60:Cz:128:LEU:HD12 | 60:Cz:131:ALA:HB3  | 1.93                     | 0.49              |
| 62:A5:377:U:N3     | 62:A5:1120:A:N1    | 2.60                     | 0.49              |
| 62:A5:2217:A:O2'   | 62:A5:3450:G:OP1   | 2.31                     | 0.49              |
| 62:A5:2542:C:O2'   | 62:A5:2543:C:O4'   | 2.30                     | 0.49              |
| 62:A5:2661:G:O2'   | 62:A5:2663:C:N4    | 2.43                     | 0.49              |
| 62:A5:3591:A:O2'   | 62:A5:3592:C:O5'   | 2.28                     | 0.49              |
| 62:A5:3715:U:O4    | 62:A5:3766:U:N3    | 2.34                     | 0.49              |
| 62:A5:3925:G:OP1   | 75:AI:172:ARG:NH1  | 2.45                     | 0.49              |
| 73:AG:78:LYS:HG3   | 73:AG:81:HIS:HE1   | 1.77                     | 0.49              |
| 75:AI:62:THR:O     | 75:AI:187:SER:OG   | 2.29                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:21:ALA:HB1    | 1:AA:170:SER:HA    | 1.94                     | 0.49              |
| 2:CA:234:LYS:HB3   | 2:CA:238:ILE:HG12  | 1.95                     | 0.49              |
| 6:CC:355:LEU:HA    | 6:CC:358:ALA:HB3   | 1.93                     | 0.49              |
| 7:Ag:215:SER:OG    | 7:Ag:234:ASN:N     | 2.45                     | 0.49              |
| 8:AU:28:SER:HB3    | 8:AU:34:LEU:HG     | 1.93                     | 0.49              |
| 9:AO:50:ARG:O      | 61:B2:1005:G:N2    | 2.38                     | 0.49              |
| 10:AX:48:LYS:HB2   | 61:B2:440:U:H5'    | 1.93                     | 0.49              |
| 12:AS:98:LEU:HB2   | 12:AS:103:LEU:HG   | 1.93                     | 0.49              |
| 17:AP:43:ARG:NH2   | 61:B2:1744:U:O4    | 2.45                     | 0.49              |
| 26:AJ:20:PRO:O     | 26:AJ:25:ARG:NH1   | 2.45                     | 0.49              |
| 32:CR:11:ALA:HA    | 32:CR:14:VAL:HG12  | 1.94                     | 0.49              |
| 34:CT:55:LYS:NZ    | 62:A5:3256:U:O3'   | 2.44                     | 0.49              |
| 34:CT:140:PHE:HA   | 71:CF:85:TYR:HA    | 1.93                     | 0.49              |
| 35:CP:174:LYS:HZ3  | 35:CP:178:GLN:HE22 | 1.58                     | 0.49              |
| 36:CX:228:ASN:O    | 36:CX:232:ALA:N    | 2.44                     | 0.49              |
| 37:CY:59:ARG:NH1   | 62:A5:216:U:OP1    | 2.45                     | 0.49              |
| 38:CZ:13:VAL:HG13  | 38:CZ:19:ALA:HA    | 1.95                     | 0.49              |
| 40:Ch:10:ARG:O     | 40:Ch:64:LYS:NZ    | 2.39                     | 0.49              |
| 53:CJ:77:CYS:SG    | 53:CJ:78:THR:N     | 2.85                     | 0.49              |
| 61:B2:714:U:OP2    | 74:AH:107:ARG:NH1  | 2.44                     | 0.49              |
| 62:A5:151:G:H2'    | 62:A5:152:A:C8     | 2.47                     | 0.49              |
| 62:A5:487:A:H61    | 62:A5:513:G:H22    | 1.58                     | 0.49              |
| 62:A5:1183:U:O2'   | 62:A5:1561:G:OP1   | 2.30                     | 0.49              |
| 62:A5:2134:A:H2'   | 62:A5:2136:U:H1'   | 1.94                     | 0.49              |
| 62:A5:2159:C:H2'   | 62:A5:2160:C:H6    | 1.78                     | 0.49              |
| 62:A5:3470:G:H2'   | 62:A5:3471:A:H8    | 1.77                     | 0.49              |
| 62:A5:3907:G:H21   | 62:A5:3944:A:H62   | 1.59                     | 0.49              |
| 64:AW:53:VAL:HG23  | 74:AH:141:ARG:HG2  | 1.95                     | 0.49              |
| 72:AE:126:VAL:HG12 | 72:AE:141:THR:HA   | 1.93                     | 0.49              |
| 4:CB:151:ARG:HA    | 4:CB:154:LEU:HB2   | 1.95                     | 0.49              |
| 6:CC:196:ARG:NH2   | 59:A8:20:C:OP2     | 2.46                     | 0.49              |
| 27:Ca:58:GLY:O     | 62:A5:3319:A:O2'   | 2.18                     | 0.49              |
| 28:CN:38:ARG:NH1   | 57:A9:16:U:OP1     | 2.44                     | 0.49              |
| 29:CI:47:PRO:HB2   | 29:CI:178:ARG:HH12 | 1.77                     | 0.49              |
| 34:CT:142:LYS:HB2  | 71:CF:83:GLN:HG2   | 1.94                     | 0.49              |
| 35:CP:6:ARG:NH2    | 35:CP:116:HIS:O    | 2.46                     | 0.49              |
| 38:CZ:134:ARG:NH2  | 62:A5:3002:U:O5'   | 2.39                     | 0.49              |
| 45:Cf:28:LYS:HG3   | 45:Cf:37:ALA:HB3   | 1.94                     | 0.49              |
| 55:CE:236:GLN:NE2  | 80:CM:104:LEU:O    | 2.41                     | 0.49              |
| 61:B2:905:U:O2     | 61:B2:938:G:N2     | 2.33                     | 0.49              |
| 61:B2:1447:G:O6    | 61:B2:1536:A:N6    | 2.46                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 61:B2:1552:C:N4    | 61:B2:1558:A:OP1   | 2.45                     | 0.49              |
| 62:A5:202:A:N1     | 62:A5:233:A:O2'    | 2.41                     | 0.49              |
| 62:A5:988:C:H2'    | 62:A5:989:A:C8     | 2.47                     | 0.49              |
| 62:A5:1223:G:H22   | 62:A5:1253:A:H2    | 1.60                     | 0.49              |
| 62:A5:1403:C:OP1   | 62:A5:1424:G:N2    | 2.45                     | 0.49              |
| 62:A5:1568:A:OP1   | 71:CF:28:GLN:NE2   | 2.44                     | 0.49              |
| 62:A5:3551:U:H2'   | 62:A5:3552:G:C8    | 2.48                     | 0.49              |
| 67:CU:211:PHE:HA   | 67:CU:214:TYR:HB2  | 1.93                     | 0.49              |
| 77:CO:21:LEU:HD22  | 77:CO:82:PHE:HZ    | 1.77                     | 0.49              |
| 77:CO:40:CYS:HB3   | 77:CO:108:ASP:HB3  | 1.94                     | 0.49              |
| 7:Ag:264:CYS:SG    | 7:Ag:265:LYS:N     | 2.86                     | 0.49              |
| 14:AN:87:ASP:N     | 14:AN:87:ASP:OD1   | 2.40                     | 0.49              |
| 23:AD:107:LEU:HA   | 23:AD:110:LYS:HB2  | 1.95                     | 0.49              |
| 28:CN:4:TYR:HA     | 28:CN:7:MET:HG2    | 1.95                     | 0.49              |
| 28:CN:162:ARG:NH1  | 62:A5:66:A:OP1     | 2.41                     | 0.49              |
| 30:CD:54:ARG:NH2   | 30:CD:147:ASP:OD2  | 2.41                     | 0.49              |
| 31:CQ:80:ILE:O     | 31:CQ:101:CYS:N    | 2.36                     | 0.49              |
| 34:CT:42:ILE:HD11  | 34:CT:74:VAL:HG21  | 1.93                     | 0.49              |
| 37:CY:80:VAL:HG12  | 37:CY:101:PRO:HD3  | 1.94                     | 0.49              |
| 53:CJ:145:ASN:OD1  | 58:A7:42:A:O2'     | 2.31                     | 0.49              |
| 61:B2:862:C:H5'    | 61:B2:863:A:H3'    | 1.94                     | 0.49              |
| 61:B2:1715:G:C6    | 69:AT:67:ARG:CD    | 2.83                     | 0.49              |
| 62:A5:1043:G:H1    | 62:A5:1050:C:H42   | 1.60                     | 0.49              |
| 62:A5:1282:U:H2'   | 62:A5:1283:A:H8    | 1.76                     | 0.49              |
| 62:A5:1978:G:H2'   | 62:A5:1979:A:H8    | 1.76                     | 0.49              |
| 62:A5:2523:A:OP1   | 62:A5:2701:G:N2    | 2.45                     | 0.49              |
| 62:A5:2742:G:H5''  | 62:A5:2742:G:H8    | 1.78                     | 0.49              |
| 62:A5:3639:U:OP2   | 62:A5:3662:G:N1    | 2.32                     | 0.49              |
| 67:CU:242:LEU:HD12 | 67:CU:244:ILE:HD11 | 1.93                     | 0.49              |
| 69:AT:129:ARG:CG   | 69:AT:133:ARG:NE   | 2.65                     | 0.49              |
| 72:AE:8:HIS:HB3    | 72:AE:27:PHE:HE1   | 1.78                     | 0.49              |
| 76:AQ:83:ILE:HG22  | 76:AQ:87:ARG:HH12  | 1.78                     | 0.49              |
| 79:CV:19:GLY:H     | 79:CV:56:GLY:HA2   | 1.78                     | 0.49              |
| 12:AS:65:ASP:OD1   | 12:AS:65:ASP:N     | 2.43                     | 0.49              |
| 17:AP:84:ARG:NH2   | 61:B2:1645:G:O2'   | 2.46                     | 0.49              |
| 17:AP:127:LYS:HD3  | 61:B2:1270:U:H5''  | 1.93                     | 0.49              |
| 18:AV:10:ASP:OD1   | 18:AV:10:ASP:N     | 2.45                     | 0.49              |
| 41:Cb:22:LYS:NZ    | 62:A5:1320:U:OP2   | 2.30                     | 0.49              |
| 43:Cd:20:ARG:HA    | 43:Cd:118:ASN:HA   | 1.95                     | 0.49              |
| 53:CJ:106:SER:HA   | 53:CJ:164:LYS:HB2  | 1.95                     | 0.49              |
| 55:CE:20:HIS:CE1   | 55:CE:31:LEU:HB3   | 2.47                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 61:B2:405:A:H4'   | 61:B2:406:A:H5'   | 1.93                     | 0.49              |
| 61:B2:961:U:O2    | 61:B2:1041:G:N1   | 2.45                     | 0.49              |
| 61:B2:1671:U:C4   | 69:AT:82:ARG:NH2  | 2.81                     | 0.49              |
| 62:A5:1083:A:N7   | 62:A5:1121:A:N6   | 2.60                     | 0.49              |
| 62:A5:2784:C:N4   | 62:A5:3346:G:O6   | 2.45                     | 0.49              |
| 62:A5:3672:U:H2'  | 62:A5:3673:G:H8   | 1.77                     | 0.49              |
| 64:AW:44:HIS:NE2  | 64:AW:112:ASP:OD2 | 2.44                     | 0.49              |
| 68:AK:27:PHE:HA   | 68:AK:41:LEU:HD13 | 1.94                     | 0.49              |
| 69:AT:133:ARG:O   | 69:AT:137:GLN:N   | 2.44                     | 0.49              |
| 78:CL:15:LYS:H    | 78:CL:17:TRP:HD1  | 1.59                     | 0.49              |
| 79:CV:17:SER:HG   | 79:CV:86:LYS:HZ1  | 1.55                     | 0.49              |
| 1:AA:34:MET:HG2   | 1:AA:150:THR:HA   | 1.94                     | 0.49              |
| 4:CB:372:SER:OG   | 4:CB:374:MET:N    | 2.44                     | 0.49              |
| 5:AC:149:ARG:H    | 5:AC:230:THR:HG21 | 1.78                     | 0.49              |
| 6:CC:269:THR:OG1  | 6:CC:270:TRP:N    | 2.44                     | 0.49              |
| 8:AU:95:SER:HB3   | 8:AU:99:ILE:HD12  | 1.94                     | 0.49              |
| 23:AD:135:GLY:HA2 | 23:AD:157:GLY:HA3 | 1.94                     | 0.49              |
| 26:AJ:143:VAL:HA  | 61:B2:849:U:H6    | 1.78                     | 0.49              |
| 28:CN:85:LYS:HG2  | 62:A5:48:U:H5'    | 1.95                     | 0.49              |
| 53:CJ:13:ALA:HB1  | 53:CJ:18:ARG:HH12 | 1.77                     | 0.49              |
| 61:B2:1670:G:P    | 69:AT:43:LYS:HZ1  | 2.35                     | 0.49              |
| 62:A5:1811:A:H62  | 62:A5:1859:U:H5'  | 1.78                     | 0.49              |
| 62:A5:2171:U:H2'  | 62:A5:2172:C:H6   | 1.77                     | 0.49              |
| 62:A5:2490:G:N2   | 62:A5:3618:A:O4'  | 2.46                     | 0.49              |
| 62:A5:3775:A:H1'  | 62:A5:3777:U:H5'  | 1.94                     | 0.49              |
| 68:AK:43:VAL:HA   | 68:AK:47:MET:HG2  | 1.95                     | 0.49              |
| 69:AT:61:LEU:CB   | 69:AT:65:TYR:HE2  | 2.23                     | 0.49              |
| 71:CF:197:GLU:HG2 | 71:CF:204:ASN:HB2 | 1.95                     | 0.49              |
| 2:CA:199:VAL:HG11 | 62:A5:1114:A:C8   | 2.48                     | 0.49              |
| 4:CB:251:VAL:HG21 | 4:CB:267:ALA:HB3  | 1.95                     | 0.49              |
| 6:CC:112:ARG:HA   | 62:A5:814:U:H5'   | 1.95                     | 0.49              |
| 22:Ab:67:THR:OG1  | 22:Ab:68:GLY:N    | 2.46                     | 0.49              |
| 28:CN:72:LYS:NZ   | 62:A5:2546:G:OP1  | 2.40                     | 0.49              |
| 30:CD:272:LYS:NZ  | 58:A7:109:U:O5'   | 2.41                     | 0.49              |
| 35:CP:104:CYS:HG  | 62:A5:399:C:HO2'  | 1.57                     | 0.49              |
| 40:Ch:53:ALA:HA   | 40:Ch:56:ARG:HD2  | 1.95                     | 0.49              |
| 45:Cf:49:ARG:HD3  | 55:CE:231:ALA:HA  | 1.95                     | 0.49              |
| 59:A8:108:A:N7    | 83:Cj:29:LEU:CD2  | 2.76                     | 0.49              |
| 61:B2:598:C:H2'   | 61:B2:599:A:C8    | 2.48                     | 0.49              |
| 61:B2:1213:A:C5   | 61:B2:1214:A:H1'  | 2.47                     | 0.49              |
| 62:A5:163:A:H8    | 62:A5:164:U:H5    | 1.61                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 62:A5:1287:U:O4    | 62:A5:1298:A:N6    | 2.41                     | 0.49              |
| 62:A5:1362:G:N1    | 62:A5:1363:G:O6    | 2.46                     | 0.49              |
| 62:A5:1562:U:H3    | 62:A5:1598:A:H61   | 1.59                     | 0.49              |
| 62:A5:1624:G:O6    | 62:A5:1664:C:N4    | 2.45                     | 0.49              |
| 62:A5:2709:U:O4    | 62:A5:2710:A:N6    | 2.46                     | 0.49              |
| 62:A5:3739:U:O2'   | 62:A5:3741:A:N7    | 2.40                     | 0.49              |
| 4:CB:261:ARG:HD3   | 77:CO:66:VAL:HG21  | 1.95                     | 0.49              |
| 6:CC:299:GLU:OE1   | 62:A5:1564:G:N2    | 2.46                     | 0.49              |
| 7:Ag:237:ILE:HG22  | 7:Ag:253:TYR:HB3   | 1.94                     | 0.49              |
| 7:Ag:243:SER:HB2   | 7:Ag:248:TRP:HE3   | 1.78                     | 0.49              |
| 9:AO:42:VAL:HG11   | 9:AO:81:VAL:HG21   | 1.95                     | 0.49              |
| 12:AS:138:THR:OG1  | 12:AS:139:THR:N    | 2.46                     | 0.49              |
| 30:CD:167:VAL:HG12 | 30:CD:173:ILE:HD13 | 1.95                     | 0.49              |
| 31:CQ:100:VAL:HB   | 31:CQ:120:VAL:HG23 | 1.93                     | 0.49              |
| 33:CS:29:LYS:NZ    | 33:CS:30:MET:O     | 2.45                     | 0.49              |
| 47:Ck:39:SER:OG    | 47:Ck:40:ARG:N     | 2.45                     | 0.49              |
| 59:A8:117:C:H2'    | 59:A8:118:A:H8     | 1.77                     | 0.49              |
| 61:B2:332:U:O4     | 61:B2:342:G:N2     | 2.46                     | 0.49              |
| 61:B2:390:A:OP2    | 72:AE:3:ARG:NH2    | 2.46                     | 0.49              |
| 61:B2:1742:A:N6    | 61:B2:1752:U:O4    | 2.46                     | 0.49              |
| 62:A5:1613:A:N6    | 62:A5:1614:A:H62   | 2.11                     | 0.49              |
| 72:AE:64:ILE:HG13  | 72:AE:69:LEU:HD13  | 1.94                     | 0.49              |
| 79:CV:32:THR:HG21  | 79:CV:114:GLY:HA2  | 1.95                     | 0.49              |
| 2:CA:226:LYS:HD3   | 2:CA:229:THR:HB    | 1.94                     | 0.48              |
| 3:AB:27:ARG:HH21   | 3:AB:51:ARG:HD3    | 1.78                     | 0.48              |
| 4:CB:224:LYS:HZ3   | 62:A5:3624:C:P     | 2.36                     | 0.48              |
| 7:Ag:17:TRP:HB2    | 7:Ag:36:ARG:HG3    | 1.94                     | 0.48              |
| 7:Ag:79:ALA:N      | 7:Ag:91:TRP:O      | 2.42                     | 0.48              |
| 17:AP:56:PRO:HB2   | 17:AP:59:LEU:HB3   | 1.95                     | 0.48              |
| 17:AP:58:ALA:O     | 17:AP:62:LYS:N     | 2.46                     | 0.48              |
| 22:Ab:33:MET:HB2   | 22:Ab:79:PHE:HB2   | 1.95                     | 0.48              |
| 25:Af:120:GLU:OE1  | 25:Af:130:VAL:N    | 2.46                     | 0.48              |
| 28:CN:71:ARG:HH22  | 62:A5:37:G:P       | 2.35                     | 0.48              |
| 33:CS:158:VAL:HA   | 80:CM:53:ASN:HB3   | 1.94                     | 0.48              |
| 54:CH:153:SER:O    | 54:CH:157:ALA:N    | 2.46                     | 0.48              |
| 55:CE:59:LYS:HA    | 55:CE:62:ILE:HB    | 1.94                     | 0.48              |
| 61:B2:221:C:O2'    | 61:B2:923:G:N1     | 2.45                     | 0.48              |
| 61:B2:1121:C:H2'   | 61:B2:1122:A:H8    | 1.78                     | 0.48              |
| 61:B2:1805:U:OP1   | 70:AF:95:ARG:NH1   | 2.46                     | 0.48              |
| 62:A5:822:G:H22    | 62:A5:991:A:H1'    | 1.78                     | 0.48              |
| 62:A5:995:G:H21    | 62:A5:1324:C:P     | 2.36                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 62:A5:1408:A:O2'  | 62:A5:1513:C:OP1  | 2.30                     | 0.48              |
| 62:A5:2178:U:H2'  | 62:A5:2179:G:O4'  | 2.13                     | 0.48              |
| 62:A5:3163:U:H2'  | 62:A5:3164:C:H6   | 1.77                     | 0.48              |
| 62:A5:3321:A:H2'  | 62:A5:3322:A:C8   | 2.47                     | 0.48              |
| 64:AW:52:ILE:HG13 | 64:AW:61:ILE:HG23 | 1.95                     | 0.48              |
| 66:Cg:94:LEU:O    | 66:Cg:98:GLN:N    | 2.38                     | 0.48              |
| 76:AQ:52:LYS:HE3  | 76:AQ:119:ARG:HB3 | 1.94                     | 0.48              |
| 4:CB:63:PRO:O     | 4:CB:65:SER:N     | 2.46                     | 0.48              |
| 8:AU:32:ARG:NH1   | 8:AU:35:GLU:OE2   | 2.45                     | 0.48              |
| 17:AP:50:ARG:NH2  | 61:B2:1745:G:OP2  | 2.44                     | 0.48              |
| 19:AY:45:LEU:HD11 | 19:AY:56:VAL:HG11 | 1.95                     | 0.48              |
| 23:AD:44:THR:OG1  | 23:AD:47:ARG:O    | 2.24                     | 0.48              |
| 25:Af:150:PHE:HA  | 25:Af:152:LYS:HD3 | 1.94                     | 0.48              |
| 31:CQ:179:GLY:O   | 31:CQ:188:LYS:N   | 2.46                     | 0.48              |
| 44:Ce:29:LYS:N    | 62:A5:805:C:OP1   | 2.46                     | 0.48              |
| 45:Cf:140:PRO:HB3 | 62:A5:449:U:H5'   | 1.96                     | 0.48              |
| 47:Ck:12:LEU:O    | 47:Ck:16:ARG:NH1  | 2.46                     | 0.48              |
| 54:CH:70:THR:O    | 54:CH:74:HIS:N    | 2.44                     | 0.48              |
| 55:CE:220:LYS:HD2 | 80:CM:109:ARG:H   | 1.78                     | 0.48              |
| 56:CG:225:GLU:HA  | 56:CG:228:LYS:HD3 | 1.95                     | 0.48              |
| 58:A7:73:U:O4     | 58:A7:74:A:N6     | 2.46                     | 0.48              |
| 61:B2:160:G:OP2   | 61:B2:160:G:N2    | 2.34                     | 0.48              |
| 61:B2:720:G:N2    | 61:B2:817:C:O2    | 2.46                     | 0.48              |
| 62:A5:88:U:H5''   | 62:A5:89:A:H5''   | 1.95                     | 0.48              |
| 62:A5:221:C:H2'   | 62:A5:228:C:H5''  | 1.95                     | 0.48              |
| 62:A5:309:C:H2'   | 62:A5:310:A:C8    | 2.48                     | 0.48              |
| 62:A5:711:A:H2    | 62:A5:725:U:H3    | 1.61                     | 0.48              |
| 62:A5:1770:C:H42  | 62:A5:2149:G:H1   | 1.60                     | 0.48              |
| 62:A5:1776:U:H1'  | 62:A5:2111:A:H2   | 1.78                     | 0.48              |
| 62:A5:3010:U:H3   | 62:A5:3107:G:H1   | 1.61                     | 0.48              |
| 62:A5:3533:U:HO2' | 62:A5:3968:C:HO2' | 1.59                     | 0.48              |
| 62:A5:3624:C:N3   | 62:A5:3625:U:N3   | 2.61                     | 0.48              |
| 62:A5:3668:G:O2'  | 77:CO:150:HIS:NE2 | 2.37                     | 0.48              |
| 62:A5:3839:A:O2'  | 62:A5:3841:C:O5'  | 2.27                     | 0.48              |
| 62:A5:3874:A:N6   | 62:A5:3888:U:O4   | 2.45                     | 0.48              |
| 62:A5:3896:G:H2'  | 62:A5:3897:G:H8   | 1.78                     | 0.48              |
| 66:Cg:40:THR:OG1  | 66:Cg:41:VAL:N    | 2.45                     | 0.48              |
| 70:AF:73:LEU:HD23 | 76:AQ:51:TYR:HB2  | 1.93                     | 0.48              |
| 74:AH:7:ILE:HG23  | 74:AH:8:ILE:HG12  | 1.95                     | 0.48              |
| 83:Cj:19:CYS:HB2  | 83:Cj:27:TYR:HB2  | 1.95                     | 0.48              |
| 2:CA:196:TRP:HH2  | 62:A5:1112:G:P    | 2.36                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 3:AB:147:ALA:HA    | 3:AB:211:HIS:HD2   | 1.78                     | 0.48              |
| 4:CB:196:TRP:O     | 4:CB:200:HIS:ND1   | 2.34                     | 0.48              |
| 4:CB:277:ARG:NH1   | 62:A5:3582:A:OP1   | 2.46                     | 0.48              |
| 5:AC:189:SER:OG    | 5:AC:190:ALA:O     | 2.32                     | 0.48              |
| 7:Ag:217:ALA:HB3   | 7:Ag:231:LEU:HB2   | 1.95                     | 0.48              |
| 10:AX:13:HIS:ND1   | 10:AX:13:HIS:O     | 2.46                     | 0.48              |
| 15:AL:56:LYS:NZ    | 61:B2:332:U:OP2    | 2.36                     | 0.48              |
| 21:Aa:74:CYS:SG    | 21:Aa:75:VAL:N     | 2.82                     | 0.48              |
| 25:Af:117:LEU:HD23 | 25:Af:118:ARG:HG2  | 1.94                     | 0.48              |
| 26:AJ:18:ARG:NH1   | 61:B2:374:C:OP1    | 2.45                     | 0.48              |
| 49:Cm:88:LYS:HA    | 49:Cm:92:ASP:HB2   | 1.95                     | 0.48              |
| 58:A7:70:G:H2'     | 58:A7:71:G:C8      | 2.49                     | 0.48              |
| 60:Cz:63:MET:HE1   | 60:Cz:108:ASP:HB2  | 1.95                     | 0.48              |
| 61:B2:124:U:H3'    | 73:AG:199:ARG:HH22 | 1.77                     | 0.48              |
| 61:B2:1452:U:O4    | 61:B2:1532:C:N4    | 2.46                     | 0.48              |
| 62:A5:444:C:N4     | 62:A5:784:G:O6     | 2.46                     | 0.48              |
| 62:A5:1875:G:O2'   | 62:A5:2111:A:N6    | 2.47                     | 0.48              |
| 62:A5:2578:U:H2'   | 62:A5:2579:G:H8    | 1.79                     | 0.48              |
| 62:A5:2933:A:N6    | 62:A5:2982:U:OP1   | 2.46                     | 0.48              |
| 62:A5:3258:C:H42   | 62:A5:3260:G:N2    | 2.11                     | 0.48              |
| 62:A5:3348:G:N3    | 62:A5:3402:C:N4    | 2.61                     | 0.48              |
| 62:A5:3370:A:N6    | 62:A5:3382:G:O2'   | 2.47                     | 0.48              |
| 64:AW:52:ILE:O     | 74:AH:142:ILE:N    | 2.41                     | 0.48              |
| 69:AT:30:VAL:HG13  | 69:AT:31:PRO:CD    | 2.43                     | 0.48              |
| 70:AF:85:PHE:O     | 70:AF:89:GLN:NE2   | 2.39                     | 0.48              |
| 4:CB:189:SER:OG    | 4:CB:191:GLU:OE1   | 2.31                     | 0.48              |
| 5:AC:232:ALA:HA    | 18:AV:23:ILE:HG21  | 1.94                     | 0.48              |
| 6:CC:70:TRP:HE1    | 6:CC:74:ARG:CZ     | 2.25                     | 0.48              |
| 12:AS:133:GLY:HA2  | 61:B2:1750:U:H4'   | 1.95                     | 0.48              |
| 28:CN:111:GLY:O    | 62:A5:24:G:O2'     | 2.26                     | 0.48              |
| 29:CI:60:LEU:O     | 29:CI:127:ALA:N    | 2.42                     | 0.48              |
| 33:CS:83:ARG:NH1   | 33:CS:91:HIS:O     | 2.46                     | 0.48              |
| 35:CP:7:GLU:HG2    | 35:CP:16:LYS:HE2   | 1.95                     | 0.48              |
| 39:Cr:120:ALA:O    | 39:Cr:124:SER:N    | 2.47                     | 0.48              |
| 42:Cc:80:GLU:O     | 42:Cc:84:ALA:N     | 2.46                     | 0.48              |
| 58:A7:97:G:H2'     | 58:A7:98:G:H8      | 1.79                     | 0.48              |
| 61:B2:1151:G:H2'   | 61:B2:1152:G:C8    | 2.48                     | 0.48              |
| 62:A5:852:C:H2'    | 62:A5:853:G:H8     | 1.78                     | 0.48              |
| 62:A5:906:A:H2'    | 62:A5:907:A:H8     | 1.78                     | 0.48              |
| 62:A5:1066:A:H1'   | 62:A5:1725:A:C8    | 2.48                     | 0.48              |
| 62:A5:1252:U:H2'   | 62:A5:1253:A:C8    | 2.49                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 62:A5:3914:G:H1    | 62:A5:3938:C:H42   | 1.59                     | 0.48              |
| 72:AE:122:LYS:HZ3  | 72:AE:145:ARG:HH21 | 1.60                     | 0.48              |
| 72:AE:194:THR:N    | 72:AE:211:LYS:O    | 2.37                     | 0.48              |
| 3:AB:126:ALA:O     | 3:AB:142:CYS:N     | 2.46                     | 0.48              |
| 6:CC:163:LYS:HG2   | 6:CC:218:GLU:HG3   | 1.95                     | 0.48              |
| 7:Ag:298:THR:HA    | 7:Ag:312:GLN:HA    | 1.96                     | 0.48              |
| 17:AP:62:LYS:NZ    | 61:B2:1329:A:OP1   | 2.46                     | 0.48              |
| 25:Af:140:TYR:OH   | 61:B2:1338:U:O2    | 2.30                     | 0.48              |
| 28:CN:24:ARG:HH12  | 62:A5:2813:G:H4'   | 1.78                     | 0.48              |
| 42:Cc:37:THR:HA    | 42:Cc:40:GLN:HG2   | 1.96                     | 0.48              |
| 49:Cm:87:GLN:HB2   | 49:Cm:91:CYS:HB2   | 1.94                     | 0.48              |
| 55:CE:222:PHE:H    | 55:CE:225:TYR:HB2  | 1.79                     | 0.48              |
| 61:B2:1053:A:H2'   | 61:B2:1054:A:C8    | 2.49                     | 0.48              |
| 61:B2:1726:A:N3    | 61:B2:1727:U:N3    | 2.62                     | 0.48              |
| 62:A5:863:U:O2'    | 62:A5:921:C:OP1    | 2.29                     | 0.48              |
| 63:Ac:13:VAL:HA    | 63:Ac:26:VAL:HG23  | 1.96                     | 0.48              |
| 72:AE:182:MET:N    | 72:AE:226:PHE:O    | 2.46                     | 0.48              |
| 73:AG:137:ARG:HG2  | 73:AG:140:LYS:H    | 1.79                     | 0.48              |
| 74:AH:67:GLN:HA    | 74:AH:70:PHE:HB2   | 1.95                     | 0.48              |
| 74:AH:174:VAL:HA   | 74:AH:177:LYS:HB2  | 1.96                     | 0.48              |
| 76:AQ:17:ARG:HA    | 76:AQ:21:ALA:HB3   | 1.94                     | 0.48              |
| 80:CM:155:LYS:HA   | 80:CM:156:ALA:HA   | 1.55                     | 0.48              |
| 2:CA:152:SER:OG    | 2:CA:154:ALA:N     | 2.44                     | 0.48              |
| 13:Ad:30:LEU:HD11  | 13:Ad:37:ASN:HA    | 1.95                     | 0.48              |
| 13:Ad:56:ASP:OXT   | 61:B2:1610:A:O2'   | 2.28                     | 0.48              |
| 14:AN:15:ALA:H     | 61:B2:1046:U:H5'   | 1.79                     | 0.48              |
| 16:AR:28:PHE:HA    | 16:AR:55:THR:HG21  | 1.94                     | 0.48              |
| 27:Ca:5:LYS:O      | 27:Ca:11:LYS:NZ    | 2.42                     | 0.48              |
| 33:CS:93:MET:SD    | 62:A5:1428:G:O2'   | 2.70                     | 0.48              |
| 33:CS:95:ARG:NH1   | 62:A5:1427:G:O2'   | 2.46                     | 0.48              |
| 35:CP:174:LYS:O    | 62:A5:3776:A:N6    | 2.47                     | 0.48              |
| 36:CX:250:ARG:HH21 | 36:CX:256:LYS:HD3  | 1.77                     | 0.48              |
| 53:CJ:18:ARG:O     | 53:CJ:141:ARG:NH1  | 2.47                     | 0.48              |
| 54:CH:51:ARG:NH2   | 62:A5:592:G:OP1    | 2.46                     | 0.48              |
| 56:CG:156:LYS:O    | 56:CG:158:GLN:NE2  | 2.46                     | 0.48              |
| 61:B2:40:A:H61     | 61:B2:472:G:H1'    | 1.79                     | 0.48              |
| 61:B2:546:A:OP2    | 61:B2:551:C:N4     | 2.34                     | 0.48              |
| 61:B2:1043:U:O2'   | 61:B2:1134:G:N3    | 2.46                     | 0.48              |
| 62:A5:389:G:O2'    | 62:A5:414:A:N6     | 2.46                     | 0.48              |
| 62:A5:1446:A:N6    | 62:A5:1492:C:OP2   | 2.43                     | 0.48              |
| 62:A5:2214:G:H21   | 79:CV:21:PRO:HG2   | 1.79                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 62:A5:2717:C:P     | 79:CV:48:ARG:HH21  | 2.36                     | 0.48              |
| 62:A5:3584:C:H42   | 62:A5:3626:A:H62   | 1.62                     | 0.48              |
| 71:CF:133:ILE:O    | 71:CF:137:ARG:N    | 2.45                     | 0.48              |
| 73:AG:209:ASP:O    | 73:AG:212:LYS:NZ   | 2.47                     | 0.48              |
| 77:CO:67:ASN:O     | 77:CO:69:ALA:N     | 2.46                     | 0.48              |
| 78:CL:83:ALA:HB1   | 78:CL:116:LEU:HD22 | 1.95                     | 0.48              |
| 80:CM:65:PRO:HG2   | 80:CM:68:ALA:HB2   | 1.95                     | 0.48              |
| 80:CM:141:ARG:O    | 80:CM:145:LYS:N    | 2.46                     | 0.48              |
| 1:AA:148:THR:OG1   | 1:AA:149:ASN:N     | 2.46                     | 0.48              |
| 2:CA:149:LYS:HB2   | 2:CA:155:LYS:HG2   | 1.96                     | 0.48              |
| 4:CB:174:ARG:HE    | 4:CB:342:LYS:HE2   | 1.79                     | 0.48              |
| 6:CC:116:ARG:NH1   | 6:CC:118:VAL:HG12  | 2.29                     | 0.48              |
| 7:Ag:49:GLU:HB3    | 7:Ag:52:ASN:H      | 1.77                     | 0.48              |
| 14:AN:7:PRO:HD3    | 61:B2:1026:A:H5'   | 1.95                     | 0.48              |
| 17:AP:21:ARG:NH1   | 17:AP:39:LEU:O     | 2.47                     | 0.48              |
| 24:Ae:110:TYR:HA   | 24:Ae:113:ARG:HB2  | 1.96                     | 0.48              |
| 26:AJ:98:VAL:HA    | 26:AJ:101:LEU:HD23 | 1.95                     | 0.48              |
| 29:CI:171:TRP:HD1  | 29:CI:178:ARG:HG3  | 1.78                     | 0.48              |
| 30:CD:211:LEU:HD13 | 30:CD:218:SER:HB2  | 1.95                     | 0.48              |
| 53:CJ:23:ARG:HG2   | 53:CJ:140:GLY:HA3  | 1.96                     | 0.48              |
| 53:CJ:89:GLU:HA    | 53:CJ:92:LEU:HG    | 1.94                     | 0.48              |
| 56:CG:166:VAL:HG21 | 56:CG:172:VAL:HG21 | 1.95                     | 0.48              |
| 58:A7:30:G:H2'     | 58:A7:31:G:H8      | 1.78                     | 0.48              |
| 61:B2:1:A:O5'      | 61:B2:375:A:OP1    | 2.31                     | 0.48              |
| 61:B2:238:C:N4     | 61:B2:239:G:O6     | 2.46                     | 0.48              |
| 61:B2:342:G:O3'    | 75:AI:10:LYS:NZ    | 2.47                     | 0.48              |
| 61:B2:947:U:O2'    | 64:AW:56:HIS:O     | 2.29                     | 0.48              |
| 61:B2:1540:G:H1    | 69:AT:129:ARG:NH2  | 2.10                     | 0.48              |
| 61:B2:1883:U:O2    | 61:B2:1903:G:N2    | 2.47                     | 0.48              |
| 62:A5:1096:A:N6    | 62:A5:2526:A:O2'   | 2.47                     | 0.48              |
| 62:A5:1324:C:OP2   | 78:CL:6:ASN:ND2    | 2.47                     | 0.48              |
| 62:A5:1630:G:O2'   | 62:A5:1659:A:N1    | 2.45                     | 0.48              |
| 62:A5:1689:G:O2'   | 62:A5:1690:U:O5'   | 2.31                     | 0.48              |
| 62:A5:1811:A:N7    | 62:A5:1859:U:O5'   | 2.45                     | 0.48              |
| 62:A5:3530:A:N6    | 62:A5:3805:U:OP2   | 2.47                     | 0.48              |
| 62:A5:3561:G:N2    | 62:A5:3564:A:OP2   | 2.38                     | 0.48              |
| 69:AT:31:PRO:C     | 69:AT:34:MET:HG2   | 2.38                     | 0.48              |
| 1:AA:34:MET:HE1    | 1:AA:37:TYR:HB2    | 1.95                     | 0.48              |
| 1:AA:61:ALA:HB2    | 1:AA:159:ILE:HD11  | 1.95                     | 0.48              |
| 1:AA:133:PRO:HA    | 1:AA:136:GLU:HB2   | 1.96                     | 0.48              |
| 1:AA:146:ALA:N     | 1:AA:159:ILE:O     | 2.46                     | 0.48              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 6:CC:2:SER:O      | 6:CC:2:SER:OG      | 2.30                     | 0.48              |
| 26:AJ:5:ARG:HD2   | 72:AE:26:VAL:HG12  | 1.95                     | 0.48              |
| 33:CS:85:ASP:HB3  | 33:CS:90:THR:HG22  | 1.95                     | 0.48              |
| 35:CP:6:ARG:CZ    | 35:CP:116:HIS:HB3  | 2.43                     | 0.48              |
| 36:CX:177:ARG:O   | 62:A5:19:C:O2'     | 2.23                     | 0.48              |
| 40:Ch:122:LYS:HG3 | 78:CL:149:LEU:HB2  | 1.96                     | 0.48              |
| 49:Cm:122:ARG:NE  | 62:A5:3379:A:OP2   | 2.44                     | 0.48              |
| 55:CE:220:LYS:HG3 | 80:CM:110:PHE:HB2  | 1.95                     | 0.48              |
| 58:A7:12:U:OP2    | 58:A7:67:G:O2'     | 2.30                     | 0.48              |
| 61:B2:108:G:O2'   | 61:B2:880:G:O6     | 2.32                     | 0.48              |
| 61:B2:1079:A:H8   | 61:B2:1972:G:H1'   | 1.79                     | 0.48              |
| 61:B2:1240:A:N6   | 61:B2:1818:U:O4    | 2.47                     | 0.48              |
| 61:B2:1303:C:N4   | 61:B2:1304:G:O6    | 2.47                     | 0.48              |
| 61:B2:1755:A:H5'  | 69:AT:41:LYS:HB3   | 1.96                     | 0.48              |
| 62:A5:355:G:O6    | 62:A5:357:C:N4     | 2.42                     | 0.48              |
| 62:A5:819:U:H2'   | 62:A5:820:A:H8     | 1.79                     | 0.48              |
| 62:A5:1017:A:H4'  | 83:Cj:13:ASN:HD21  | 1.78                     | 0.48              |
| 62:A5:1900:U:H2'  | 62:A5:1901:G:H8    | 1.79                     | 0.48              |
| 62:A5:3153:G:N2   | 81:B:73:C:OP1      | 2.47                     | 0.48              |
| 62:A5:3814:U:H2'  | 62:A5:3815:G:H8    | 1.79                     | 0.48              |
| 4:CB:139:ASP:OD1  | 4:CB:139:ASP:N     | 2.40                     | 0.48              |
| 4:CB:313:SER:OG   | 4:CB:314:ILE:N     | 2.47                     | 0.48              |
| 5:AC:97:LYS:HD3   | 61:B2:1388:U:H5'   | 1.96                     | 0.48              |
| 7:Ag:23:THR:HG21  | 7:Ag:293:SER:HA    | 1.96                     | 0.48              |
| 21:Aa:18:VAL:HG12 | 61:B2:1030:C:H41   | 1.79                     | 0.48              |
| 30:CD:274:THR:OG1 | 30:CD:275:ASN:N    | 2.46                     | 0.48              |
| 39:Cr:16:ASN:OD1  | 39:Cr:17:ALA:N     | 2.46                     | 0.48              |
| 51:Cp:44:LYS:NZ   | 62:A5:2040:A:OP1   | 2.33                     | 0.48              |
| 60:Cz:65:VAL:HG11 | 60:Cz:111:LEU:HG   | 1.96                     | 0.48              |
| 61:B2:1258:G:N2   | 61:B2:1763:C:O2'   | 2.41                     | 0.48              |
| 62:A5:3306:U:H2'  | 62:A5:3307:A:H8    | 1.77                     | 0.48              |
| 64:AW:114:GLU:HA  | 64:AW:117:ARG:HB2  | 1.95                     | 0.48              |
| 66:Cg:81:CYS:SG   | 66:Cg:84:CYS:N     | 2.87                     | 0.48              |
| 75:AI:83:TYR:HB2  | 75:AI:204:ILE:HD11 | 1.96                     | 0.48              |
| 5:AC:91:LYS:HE2   | 5:AC:216:LEU:HD13  | 1.95                     | 0.48              |
| 6:CC:300:GLU:HA   | 6:CC:303:LYS:HE2   | 1.95                     | 0.48              |
| 6:CC:376:LYS:HA   | 6:CC:379:ALA:HB3   | 1.96                     | 0.48              |
| 11:AM:96:SER:OG   | 11:AM:97:GLY:N     | 2.47                     | 0.48              |
| 16:AR:28:PHE:O    | 16:AR:32:LYS:N     | 2.37                     | 0.48              |
| 16:AR:42:PRO:HG3  | 23:AD:208:ASP:HA   | 1.96                     | 0.48              |
| 27:Ca:49:TYR:OH   | 62:A5:1167:A:OP1   | 2.32                     | 0.48              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 27:Ca:78:LYS:HA   | 31:CQ:91:ARG:HG2   | 1.96                     | 0.48              |
| 27:Ca:102:ILE:HB  | 27:Ca:125:VAL:HG23 | 1.96                     | 0.48              |
| 28:CN:179:ARG:NH1 | 62:A5:321:G:OP1    | 2.47                     | 0.48              |
| 37:CY:87:ARG:NH2  | 62:A5:411:U:O2'    | 2.47                     | 0.48              |
| 38:CZ:75:LEU:HA   | 62:A5:1948:C:H4'   | 1.94                     | 0.48              |
| 61:B2:498:U:O2'   | 61:B2:502:C:N3     | 2.41                     | 0.48              |
| 61:B2:1367:C:H2'  | 61:B2:1368:G:H8    | 1.78                     | 0.48              |
| 61:B2:1716:A:H2   | 61:B2:1782:G:H1'   | 1.79                     | 0.48              |
| 62:A5:494:U:H2'   | 62:A5:495:A:H8     | 1.79                     | 0.48              |
| 62:A5:1550:U:OP2  | 71:CF:216:LYS:NZ   | 2.37                     | 0.48              |
| 66:Cg:44:CYS:HB2  | 66:Cg:51:LEU:HD21  | 1.95                     | 0.48              |
| 66:Cg:44:CYS:SG   | 66:Cg:81:CYS:N     | 2.73                     | 0.48              |
| 69:AT:30:VAL:CG1  | 69:AT:31:PRO:HD2   | 2.44                     | 0.48              |
| 72:AE:5:PRO:HD2   | 72:AE:7:LYS:HG3    | 1.96                     | 0.48              |
| 78:CL:57:VAL:HB   | 78:CL:72:GLY:HA2   | 1.96                     | 0.48              |
| 80:CM:117:ARG:O   | 80:CM:121:LYS:N    | 2.46                     | 0.48              |
| 6:CC:104:MET:SD   | 62:A5:1670:G:N2    | 2.87                     | 0.47              |
| 7:Ag:189:HIS:CD2  | 23:AD:224:PRO:HB3  | 2.49                     | 0.47              |
| 9:AO:51:GLU:HG3   | 61:B2:982:G:H4'    | 1.95                     | 0.47              |
| 26:AJ:173:ARG:NH2 | 61:B2:543:A:OP1    | 2.47                     | 0.47              |
| 28:CN:159:ARG:NH2 | 28:CN:164:LEU:O    | 2.47                     | 0.47              |
| 30:CD:40:ASP:HB2  | 30:CD:43:LYS:HE3   | 1.96                     | 0.47              |
| 42:Cc:56:ARG:NH2  | 42:Cc:59:GLU:OE2   | 2.47                     | 0.47              |
| 48:Cl:3:ALA:O     | 48:Cl:4:HIS:ND1    | 2.47                     | 0.47              |
| 51:Cp:67:GLY:H    | 51:Cp:72:SER:HA    | 1.78                     | 0.47              |
| 56:CG:144:GLY:O   | 56:CG:147:THR:OG1  | 2.28                     | 0.47              |
| 59:A8:32:G:C8     | 62:A5:63:G:H2'     | 2.50                     | 0.47              |
| 59:A8:42:A:H2'    | 59:A8:43:A:H8      | 1.79                     | 0.47              |
| 61:B2:36:C:H42    | 61:B2:477:A:H61    | 1.62                     | 0.47              |
| 62:A5:115:U:OP1   | 78:CL:99:ARG:NH2   | 2.47                     | 0.47              |
| 62:A5:446:C:H2'   | 62:A5:447:G:C8     | 2.49                     | 0.47              |
| 62:A5:805:C:H2'   | 62:A5:806:A:C8     | 2.49                     | 0.47              |
| 62:A5:1909:U:N3   | 62:A5:2132:A:N7    | 2.62                     | 0.47              |
| 62:A5:3017:U:O2'  | 62:A5:3102:C:O2    | 2.31                     | 0.47              |
| 62:A5:3672:U:H2'  | 62:A5:3673:G:C8    | 2.49                     | 0.47              |
| 72:AE:122:LYS:HB3 | 72:AE:164:ILE:HD11 | 1.95                     | 0.47              |
| 73:AG:56:ASN:O    | 73:AG:107:SER:OG   | 2.30                     | 0.47              |
| 75:AI:177:ILE:HA  | 75:AI:189:GLY:HA3  | 1.96                     | 0.47              |
| 78:CL:90:ALA:HB1  | 78:CL:95:ILE:HG13  | 1.95                     | 0.47              |
| 83:Cj:43:LYS:HG2  | 83:Cj:43:LYS:O     | 2.14                     | 0.47              |
| 1:AA:147:PHE:HD1  | 1:AA:161:ILE:HB    | 1.78                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 6:CC:117:LYS:HB2   | 62:A5:832:U:C5     | 2.49                     | 0.47              |
| 6:CC:118:VAL:N     | 62:A5:832:U:O4     | 2.37                     | 0.47              |
| 6:CC:190:GLN:HG3   | 6:CC:206:ALA:HB2   | 1.95                     | 0.47              |
| 16:AR:11:LYS:NZ    | 61:B2:1404:C:OP1   | 2.47                     | 0.47              |
| 30:CD:29:ASP:CG    | 30:CD:32:ALA:H     | 2.22                     | 0.47              |
| 31:CQ:122:THR:N    | 31:CQ:125:GLN:OE1  | 2.39                     | 0.47              |
| 38:CZ:46:ILE:HA    | 38:CZ:70:PRO:HA    | 1.95                     | 0.47              |
| 41:Cb:73:PRO:HG2   | 62:A5:1294:U:C2    | 2.48                     | 0.47              |
| 42:Cc:90:ARG:NH2   | 62:A5:2041:G:OP2   | 2.45                     | 0.47              |
| 46:Ci:40:LYS:NZ    | 62:A5:334:U:O2     | 2.47                     | 0.47              |
| 54:CH:45:MET:HB3   | 54:CH:55:VAL:HG23  | 1.95                     | 0.47              |
| 61:B2:153:A:H61    | 61:B2:424:G:H1'    | 1.77                     | 0.47              |
| 61:B2:1184:U:H3    | 64:AW:71:LYS:HZ3   | 1.62                     | 0.47              |
| 62:A5:1073:C:N4    | 62:A5:1075:G:O6    | 2.48                     | 0.47              |
| 62:A5:1292:G:N2    | 62:A5:1296:U:OP2   | 2.47                     | 0.47              |
| 62:A5:1421:G:H22   | 62:A5:1514:U:H1'   | 1.79                     | 0.47              |
| 62:A5:3374:U:OP1   | 62:A5:3376:C:N4    | 2.48                     | 0.47              |
| 69:AT:76:THR:HA    | 69:AT:79:TYR:HB2   | 1.95                     | 0.47              |
| 71:CF:57:ALA:HA    | 71:CF:60:TYR:HB2   | 1.95                     | 0.47              |
| 1:AA:12:GLU:HA     | 1:AA:15:ILE:HD13   | 1.96                     | 0.47              |
| 8:AU:31:VAL:HA     | 8:AU:34:LEU:HB2    | 1.96                     | 0.47              |
| 10:AX:3:LYS:NZ     | 61:B2:620:U:OP2    | 2.37                     | 0.47              |
| 20:AZ:82:LEU:O     | 20:AZ:86:ALA:N     | 2.47                     | 0.47              |
| 26:AJ:39:ARG:NH2   | 61:B2:602:A:OP1    | 2.47                     | 0.47              |
| 28:CN:113:LEU:HD12 | 28:CN:134:LEU:HD13 | 1.96                     | 0.47              |
| 37:CY:39:ARG:HH22  | 37:CY:45:ARG:CZ    | 2.27                     | 0.47              |
| 38:CZ:61:LYS:NZ    | 62:A5:3104:C:OP1   | 2.44                     | 0.47              |
| 53:CJ:17:MET:HE2   | 58:A7:54:A:C6      | 2.49                     | 0.47              |
| 55:CE:198:ARG:HA   | 55:CE:201:ASP:HB2  | 1.95                     | 0.47              |
| 58:A7:75:G:O2'     | 58:A7:99:G:N1      | 2.32                     | 0.47              |
| 61:B2:188:C:O4'    | 61:B2:196:G:N2     | 2.47                     | 0.47              |
| 61:B2:466:G:H2'    | 61:B2:467:G:C8     | 2.49                     | 0.47              |
| 61:B2:1290:A:O2'   | 61:B2:1293:C:N4    | 2.47                     | 0.47              |
| 61:B2:1670:G:O2'   | 69:AT:52:TRP:CD2   | 2.65                     | 0.47              |
| 62:A5:1069:A:N1    | 62:A5:1070:G:N2    | 2.62                     | 0.47              |
| 62:A5:1159:C:H2'   | 62:A5:2788:U:H3    | 1.79                     | 0.47              |
| 62:A5:1518:A:O2'   | 62:A5:1519:A:O4'   | 2.30                     | 0.47              |
| 62:A5:2926:G:N2    | 62:A5:2992:A:O2'   | 2.48                     | 0.47              |
| 62:A5:3494:C:N4    | 62:A5:3495:G:O6    | 2.47                     | 0.47              |
| 71:CF:36:SER:HA    | 71:CF:39:ARG:HB2   | 1.95                     | 0.47              |
| 71:CF:132:THR:O    | 71:CF:136:LEU:N    | 2.44                     | 0.47              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 72:AE:99:PHE:HE1  | 72:AE:113:ARG:HG2  | 1.79                     | 0.47              |
| 72:AE:182:MET:O   | 72:AE:226:PHE:N    | 2.45                     | 0.47              |
| 73:AG:138:ALA:HA  | 73:AG:141:ILE:HG22 | 1.96                     | 0.47              |
| 1:AA:108:PHE:O    | 5:AC:72:LYS:NZ     | 2.40                     | 0.47              |
| 2:CA:230:SER:O    | 2:CA:233:ARG:N     | 2.37                     | 0.47              |
| 12:AS:38:ARG:NH1  | 61:B2:1731:U:O3'   | 2.47                     | 0.47              |
| 16:AR:104:GLU:O   | 16:AR:108:LEU:N    | 2.43                     | 0.47              |
| 20:AZ:110:ARG:NH1 | 20:AZ:111:ALA:O    | 2.48                     | 0.47              |
| 26:AJ:47:VAL:HG11 | 26:AJ:107:LEU:HD21 | 1.95                     | 0.47              |
| 29:CI:38:ARG:HB2  | 29:CI:83:ASP:HB2   | 1.94                     | 0.47              |
| 43:Cd:56:THR:OG1  | 43:Cd:99:LEU:O     | 2.29                     | 0.47              |
| 44:Ce:29:LYS:NZ   | 62:A5:805:C:OP2    | 2.40                     | 0.47              |
| 45:Cf:11:ALA:HA   | 45:Cf:14:ALA:HB3   | 1.97                     | 0.47              |
| 50:Cn:2:ARG:HB2   | 50:Cn:5:TRP:CD1    | 2.50                     | 0.47              |
| 61:B2:1566:U:O2'  | 61:B2:1569:C:OP1   | 2.32                     | 0.47              |
| 62:A5:183:U:H2'   | 62:A5:184:A:H8     | 1.78                     | 0.47              |
| 62:A5:466:U:O4    | 62:A5:467:A:N6     | 2.47                     | 0.47              |
| 62:A5:2534:G:H22  | 62:A5:2560:A:H1'   | 1.79                     | 0.47              |
| 62:A5:2744:C:N4   | 62:A5:2759:G:O6    | 2.47                     | 0.47              |
| 62:A5:3166:C:N3   | 62:A5:3167:A:N6    | 2.63                     | 0.47              |
| 62:A5:3354:U:H2'  | 62:A5:3355:G:H8    | 1.79                     | 0.47              |
| 62:A5:3476:G:O2'  | 62:A5:3479:C:OP2   | 2.23                     | 0.47              |
| 65:CW:52:THR:OG1  | 65:CW:53:VAL:N     | 2.47                     | 0.47              |
| 69:AT:76:THR:OG1  | 69:AT:97:ASP:CG    | 2.43                     | 0.47              |
| 73:AG:7:TYR:HB2   | 73:AG:124:LEU:HD23 | 1.95                     | 0.47              |
| 73:AG:136:LYS:NZ  | 73:AG:176:LYS:O    | 2.37                     | 0.47              |
| 75:AI:62:THR:OG1  | 75:AI:63:GLY:N     | 2.45                     | 0.47              |
| 81:B:48:C:H2'     | 81:B:49:G:H8       | 1.79                     | 0.47              |
| 1:AA:186:ARG:NH2  | 18:AV:48:ASP:OD1   | 2.41                     | 0.47              |
| 4:CB:62:ARG:HH12  | 4:CB:358:SER:HA    | 1.79                     | 0.47              |
| 5:AC:84:SER:O     | 5:AC:84:SER:OG     | 2.30                     | 0.47              |
| 5:AC:89:VAL:HA    | 5:AC:111:VAL:HG23  | 1.97                     | 0.47              |
| 5:AC:166:LYS:HD2  | 64:AW:95:PRO:HA    | 1.95                     | 0.47              |
| 7:Ag:176:LYS:HE2  | 7:Ag:188:ASN:HA    | 1.96                     | 0.47              |
| 17:AP:47:ARG:HD3  | 17:AP:87:ILE:HD11  | 1.97                     | 0.47              |
| 19:AY:65:PHE:HB3  | 26:AJ:142:VAL:HG23 | 1.95                     | 0.47              |
| 20:AZ:100:VAL:HB  | 20:AZ:107:ILE:H    | 1.79                     | 0.47              |
| 27:Ca:52:GLY:O    | 31:CQ:176:ARG:N    | 2.47                     | 0.47              |
| 40:Ch:97:PRO:O    | 40:Ch:101:ASN:OD1  | 2.33                     | 0.47              |
| 55:CE:218:GLU:OE1 | 55:CE:225:TYR:OH   | 2.30                     | 0.47              |
| 59:A8:6:U:H2'     | 59:A8:7:A:H8       | 1.80                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 61:B2:922:G:H2'   | 61:B2:923:G:H8    | 1.80                     | 0.47              |
| 61:B2:1088:A:OP1  | 81:B:37:A:O2'     | 2.32                     | 0.47              |
| 61:B2:1291:A:H3'  | 61:B2:1292:A:H8   | 1.78                     | 0.47              |
| 61:B2:1459:G:O2'  | 61:B2:1529:G:N1   | 2.42                     | 0.47              |
| 61:B2:1614:A:H2'  | 61:B2:1615:U:H6   | 1.80                     | 0.47              |
| 62:A5:186:G:H5'   | 62:A5:263:A:H61   | 1.78                     | 0.47              |
| 62:A5:716:C:OP2   | 62:A5:717:A:N6    | 2.47                     | 0.47              |
| 62:A5:1502:A:H2'  | 62:A5:1503:G:H8   | 1.80                     | 0.47              |
| 62:A5:2015:G:O2'  | 62:A5:2055:G:O6   | 2.28                     | 0.47              |
| 62:A5:2530:C:H2'  | 62:A5:2531:A:C8   | 2.49                     | 0.47              |
| 62:A5:3594:A:N6   | 62:A5:3619:U:O4   | 2.47                     | 0.47              |
| 62:A5:3800:G:N2   | 62:A5:3809:U:H3   | 2.11                     | 0.47              |
| 69:AT:29:LYS:NZ   | 69:AT:106:ALA:C   | 2.71                     | 0.47              |
| 80:CM:146:ASP:OD1 | 80:CM:146:ASP:N   | 2.46                     | 0.47              |
| 4:CB:90:VAL:HA    | 4:CB:104:ASN:HB2  | 1.97                     | 0.47              |
| 6:CC:116:ARG:HE   | 62:A5:991:A:H5'   | 1.79                     | 0.47              |
| 6:CC:317:ARG:NE   | 6:CC:318:ARG:O    | 2.37                     | 0.47              |
| 22:Ab:40:CYS:SG   | 22:Ab:61:THR:OG1  | 2.72                     | 0.47              |
| 27:Ca:12:LEU:O    | 27:Ca:15:HIS:N    | 2.36                     | 0.47              |
| 29:CI:19:LYS:HD2  | 29:CI:26:VAL:HG21 | 1.97                     | 0.47              |
| 30:CD:142:PHE:O   | 30:CD:172:ASN:ND2 | 2.37                     | 0.47              |
| 33:CS:174:THR:O   | 62:A5:3753:A:O2'  | 2.30                     | 0.47              |
| 54:CH:148:ASP:OD2 | 54:CH:151:SER:OG  | 2.29                     | 0.47              |
| 61:B2:71:G:H1     | 61:B2:78:A:H5'    | 1.80                     | 0.47              |
| 61:B2:608:U:H2'   | 61:B2:609:A:C8    | 2.49                     | 0.47              |
| 61:B2:1212:A:H2'  | 61:B2:1213:A:H8   | 1.78                     | 0.47              |
| 62:A5:1579:U:O2'  | 62:A5:1581:G:N2   | 2.47                     | 0.47              |
| 62:A5:2138:C:H2'  | 62:A5:2139:U:H6   | 1.78                     | 0.47              |
| 62:A5:3736:A:H2'  | 62:A5:3737:A:H8   | 1.79                     | 0.47              |
| 62:A5:3871:U:H3   | 62:A5:3965:A:H61  | 1.61                     | 0.47              |
| 63:Ac:9:ARG:N     | 63:Ac:29:GLU:O    | 2.46                     | 0.47              |
| 72:AE:11:ARG:NH1  | 72:AE:21:ASP:OD1  | 2.46                     | 0.47              |
| 77:CO:38:VAL:HG12 | 77:CO:107:PHE:HB2 | 1.95                     | 0.47              |
| 79:CV:13:LYS:NZ   | 79:CV:59:ASP:OD2  | 2.34                     | 0.47              |
| 79:CV:22:VAL:HA   | 79:CV:23:GLY:HA2  | 1.65                     | 0.47              |
| 80:CM:139:THR:HA  | 80:CM:141:ARG:H   | 1.79                     | 0.47              |
| 3:AB:99:VAL:HG23  | 3:AB:101:CYS:HB2  | 1.97                     | 0.47              |
| 4:CB:161:ARG:HA   | 4:CB:184:GLN:HA   | 1.96                     | 0.47              |
| 5:AC:64:ILE:HA    | 5:AC:69:LEU:HD23  | 1.95                     | 0.47              |
| 7:Ag:45:LEU:HA    | 7:Ag:54:GLY:HA2   | 1.97                     | 0.47              |
| 7:Ag:73:SER:OG    | 7:Ag:75:ASP:O     | 2.32                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:Ag:172:ASP:OD1   | 7:Ag:172:ASP:N     | 2.38                     | 0.47              |
| 7:Ag:199:VAL:HG12  | 7:Ag:210:SER:HA    | 1.97                     | 0.47              |
| 13:Ad:36:LEU:HG    | 13:Ad:38:ILE:HB    | 1.95                     | 0.47              |
| 15:AL:17:LEU:HD11  | 75:AI:195:LYS:HG2  | 1.97                     | 0.47              |
| 17:AP:96:ILE:HG12  | 17:AP:107:GLN:HG2  | 1.96                     | 0.47              |
| 19:AY:6:ALA:HB1    | 19:AY:30:HIS:HA    | 1.96                     | 0.47              |
| 20:AZ:110:ARG:HH12 | 20:AZ:113:LYS:HE2  | 1.79                     | 0.47              |
| 28:CN:165:THR:OG1  | 28:CN:166:SER:N    | 2.47                     | 0.47              |
| 29:CI:47:PRO:HD2   | 29:CI:141:SER:HA   | 1.96                     | 0.47              |
| 29:CI:148:VAL:O    | 29:CI:152:LEU:N    | 2.47                     | 0.47              |
| 30:CD:150:LEU:HD12 | 53:CJ:151:ARG:HG3  | 1.95                     | 0.47              |
| 32:CR:98:ARG:NH1   | 32:CR:132:PHE:O    | 2.47                     | 0.47              |
| 33:CS:35:PRO:HG2   | 33:CS:39:VAL:HG11  | 1.96                     | 0.47              |
| 34:CT:51:GLY:O     | 34:CT:95:HIS:NE2   | 2.36                     | 0.47              |
| 34:CT:141:VAL:O    | 71:CF:84:PHE:N     | 2.42                     | 0.47              |
| 37:CY:125:GLY:HA3  | 62:A5:200:U:H4'    | 1.96                     | 0.47              |
| 38:CZ:68:VAL:HG23  | 38:CZ:70:PRO:HD3   | 1.97                     | 0.47              |
| 45:Cf:127:ASN:OD1  | 62:A5:1541:A:O2'   | 2.31                     | 0.47              |
| 53:CJ:49:THR:HG23  | 53:CJ:51:GLN:H     | 1.79                     | 0.47              |
| 53:CJ:93:LYS:HZ3   | 53:CJ:120:LEU:HA   | 1.80                     | 0.47              |
| 54:CH:4:ILE:HG23   | 54:CH:59:PHE:HE1   | 1.80                     | 0.47              |
| 55:CE:166:ALA:HA   | 55:CE:169:ARG:HG3  | 1.97                     | 0.47              |
| 61:B2:60:U:N3      | 61:B2:63:G:OP2     | 2.38                     | 0.47              |
| 61:B2:139:U:H2'    | 61:B2:140:G:H8     | 1.80                     | 0.47              |
| 61:B2:1151:G:H2'   | 61:B2:1152:G:H8    | 1.80                     | 0.47              |
| 61:B2:1564:A:O3'   | 76:AQ:2:GLN:NE2    | 2.48                     | 0.47              |
| 61:B2:1740:G:H2'   | 61:B2:1741:A:H8    | 1.80                     | 0.47              |
| 61:B2:1783:U:P     | 69:AT:92:PHE:CD2   | 3.07                     | 0.47              |
| 61:B2:1824:C:H5'   | 61:B2:1830:G:H21   | 1.80                     | 0.47              |
| 61:B2:1992:A:O2'   | 61:B2:1993:U:O4'   | 2.33                     | 0.47              |
| 62:A5:174:A:H4'    | 78:CL:134:ARG:HH22 | 1.79                     | 0.47              |
| 62:A5:396:A:OP2    | 62:A5:397:C:N4     | 2.47                     | 0.47              |
| 62:A5:406:G:H2'    | 62:A5:407:A:H8     | 1.79                     | 0.47              |
| 62:A5:462:C:H1'    | 62:A5:537:A:H1'    | 1.96                     | 0.47              |
| 62:A5:1036:A:N6    | 62:A5:1057:G:O4'   | 2.47                     | 0.47              |
| 62:A5:1388:C:O2'   | 77:CO:89:MET:SD    | 2.69                     | 0.47              |
| 62:A5:1741:G:H22   | 62:A5:1762:G:H1'   | 1.80                     | 0.47              |
| 62:A5:2847:G:H22   | 62:A5:2870:C:H42   | 1.62                     | 0.47              |
| 62:A5:3254:U:H2'   | 62:A5:3255:G:C8    | 2.50                     | 0.47              |
| 62:A5:3339:U:O2'   | 62:A5:3341:C:OP1   | 2.28                     | 0.47              |
| 62:A5:3461:C:H2'   | 62:A5:3462:A:C8    | 2.50                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 69:AT:47:PRO:HD2   | 69:AT:47:PRO:O     | 2.15                     | 0.47              |
| 69:AT:60:ILE:CG2   | 69:AT:60:ILE:O     | 2.63                     | 0.47              |
| 69:AT:77:LYS:HE2   | 69:AT:94:ARG:HD3   | 1.97                     | 0.47              |
| 70:AF:74:PRO:O     | 70:AF:110:LYS:NZ   | 2.48                     | 0.47              |
| 70:AF:121:PHE:O    | 70:AF:125:HIS:N    | 2.48                     | 0.47              |
| 75:AI:120:PRO:HG2  | 75:AI:123:ARG:HH12 | 1.79                     | 0.47              |
| 76:AQ:4:LYS:NZ     | 76:AQ:5:ARG:O      | 2.46                     | 0.47              |
| 78:CL:62:THR:OG1   | 78:CL:63:ILE:N     | 2.41                     | 0.47              |
| 79:CV:20:LEU:HA    | 79:CV:20:LEU:HD23  | 1.78                     | 0.47              |
| 83:Cj:54:LYS:C     | 83:Cj:56:ARG:H     | 2.23                     | 0.47              |
| 4:CB:389:MET:HG2   | 62:A5:3943:G:C6    | 2.49                     | 0.47              |
| 12:AS:114:LEU:HD21 | 12:AS:121:ARG:HB2  | 1.95                     | 0.47              |
| 14:AN:73:ARG:HD2   | 61:B2:945:A:C6     | 2.50                     | 0.47              |
| 17:AP:61:LYS:HD3   | 17:AP:64:ARG:HG3   | 1.97                     | 0.47              |
| 22:Ab:7:LEU:HD21   | 64:AW:26:LEU:HD13  | 1.97                     | 0.47              |
| 25:Af:145:ASN:ND2  | 61:B2:1320:G:N3    | 2.63                     | 0.47              |
| 27:Ca:43:ARG:NH2   | 62:A5:3331:A:O2'   | 2.48                     | 0.47              |
| 32:CR:101:VAL:HG11 | 62:A5:2264:G:H5'   | 1.96                     | 0.47              |
| 34:CT:29:THR:OG1   | 34:CT:94:GLU:OE1   | 2.29                     | 0.47              |
| 51:Cp:50:ALA:O     | 62:A5:2108:U:N3    | 2.44                     | 0.47              |
| 55:CE:237:TYR:HB3  | 55:CE:239:HIS:H    | 1.80                     | 0.47              |
| 59:A8:12:G:N1      | 59:A8:13:U:O4      | 2.48                     | 0.47              |
| 61:B2:66:C:O3'     | 73:AG:160:ARG:NH2  | 2.48                     | 0.47              |
| 61:B2:999:U:O2     | 61:B2:1000:G:O2'   | 2.29                     | 0.47              |
| 61:B2:1587:U:N3    | 61:B2:1597:A:OP1   | 2.48                     | 0.47              |
| 61:B2:1667:A:N6    | 61:B2:1723:U:O4    | 2.48                     | 0.47              |
| 62:A5:1100:G:H1'   | 62:A5:1873:A:N6    | 2.29                     | 0.47              |
| 62:A5:2502:G:H2'   | 62:A5:2503:G:C8    | 2.49                     | 0.47              |
| 62:A5:3468:G:H2'   | 62:A5:3469:G:C8    | 2.50                     | 0.47              |
| 64:AW:54:ASP:HA    | 64:AW:59:GLY:HA2   | 1.97                     | 0.47              |
| 69:AT:126:ILE:HG22 | 69:AT:126:ILE:O    | 2.14                     | 0.47              |
| 69:AT:139:VAL:HA   | 69:AT:142:GLN:HB2  | 1.96                     | 0.47              |
| 77:CO:37:VAL:HG13  | 77:CO:106:VAL:HG13 | 1.96                     | 0.47              |
| 2:CA:109:GLU:OE2   | 2:CA:139:HIS:N     | 2.46                     | 0.47              |
| 4:CB:22:SER:OG     | 4:CB:23:ALA:N      | 2.47                     | 0.47              |
| 7:Ag:209:THR:HG23  | 7:Ag:240:LEU:HD13  | 1.96                     | 0.47              |
| 10:AX:4:PRO:HG2    | 10:AX:13:HIS:CD2   | 2.49                     | 0.47              |
| 11:AM:35:ALA:HB1   | 11:AM:122:GLY:HA3  | 1.95                     | 0.47              |
| 19:AY:117:LYS:HZ3  | 73:AG:87:ARG:HH22  | 1.63                     | 0.47              |
| 22:Ab:36:LYS:O     | 22:Ab:78:SER:OG    | 2.32                     | 0.47              |
| 22:Ab:67:THR:O     | 61:B2:958:G:O2'    | 2.27                     | 0.47              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 23:AD:195:ASP:OD1 | 23:AD:195:ASP:N    | 2.42                     | 0.47              |
| 29:CI:52:LEU:HD13 | 29:CI:152:LEU:HD13 | 1.97                     | 0.47              |
| 36:CX:246:ASN:HB2 | 36:CX:258:TYR:HB2  | 1.97                     | 0.47              |
| 43:Cd:25:HIS:CG   | 43:Cd:28:LYS:HB3   | 2.50                     | 0.47              |
| 52:Co:65:LYS:HE2  | 52:Co:85:ARG:HE    | 1.79                     | 0.47              |
| 53:CJ:29:ILE:HB   | 53:CJ:75:VAL:HB    | 1.97                     | 0.47              |
| 61:B2:18:C:H2'    | 61:B2:19:A:C8      | 2.50                     | 0.47              |
| 61:B2:1404:C:O2'  | 61:B2:1593:U:O2    | 2.32                     | 0.47              |
| 61:B2:1564:A:N7   | 61:B2:1565:C:O2'   | 2.43                     | 0.47              |
| 61:B2:1675:A:N3   | 61:B2:1799:A:O2'   | 2.46                     | 0.47              |
| 62:A5:1136:A:H2'  | 62:A5:1138:C:C5    | 2.50                     | 0.47              |
| 62:A5:2118:U:H2'  | 62:A5:2119:G:H8    | 1.80                     | 0.47              |
| 62:A5:2251:G:H2'  | 62:A5:2252:A:C8    | 2.50                     | 0.47              |
| 62:A5:2778:G:N2   | 62:A5:3511:U:O2    | 2.48                     | 0.47              |
| 62:A5:3304:U:H4'  | 62:A5:3305:U:H5'   | 1.96                     | 0.47              |
| 64:AW:90:THR:OG1  | 64:AW:91:ASN:N     | 2.48                     | 0.47              |
| 69:AT:134:ILE:O   | 69:AT:138:ILE:HG13 | 2.15                     | 0.47              |
| 74:AH:48:ARG:HB3  | 74:AH:59:ILE:HD13  | 1.97                     | 0.47              |
| 77:CO:151:TYR:HB3 | 77:CO:154:VAL:HB   | 1.97                     | 0.47              |
| 78:CL:37:ASN:O    | 78:CL:41:LYS:N     | 2.47                     | 0.47              |
| 2:CA:117:GLU:OE1  | 2:CA:119:LYS:N     | 2.47                     | 0.47              |
| 4:CB:2:SER:O      | 4:CB:2:SER:OG      | 2.26                     | 0.47              |
| 5:AC:205:CYS:SG   | 5:AC:207:THR:OG1   | 2.71                     | 0.47              |
| 8:AU:48:GLN:HG3   | 8:AU:50:LEU:HD23   | 1.97                     | 0.47              |
| 14:AN:109:LYS:HA  | 14:AN:112:LYS:HB3  | 1.96                     | 0.47              |
| 14:AN:117:LEU:O   | 14:AN:120:SER:OG   | 2.28                     | 0.47              |
| 20:AZ:71:VAL:HA   | 20:AZ:74:GLU:HB2   | 1.97                     | 0.47              |
| 22:Ab:20:LYS:NZ   | 61:B2:1046:U:OP2   | 2.44                     | 0.47              |
| 23:AD:199:LYS:HD2 | 23:AD:202:PRO:HG3  | 1.96                     | 0.47              |
| 26:AJ:151:ARG:O   | 26:AJ:154:SER:OG   | 2.32                     | 0.47              |
| 33:CS:15:ARG:O    | 33:CS:25:THR:OG1   | 2.25                     | 0.47              |
| 34:CT:43:LYS:NZ   | 62:A5:1205:U:OP1   | 2.32                     | 0.47              |
| 35:CP:133:HIS:N   | 62:A5:1080:G:O6    | 2.48                     | 0.47              |
| 45:Cf:137:ARG:NH1 | 62:A5:772:G:OP2    | 2.48                     | 0.47              |
| 54:CH:187:LYS:HA  | 54:CH:188:LEU:HA   | 1.61                     | 0.47              |
| 61:B2:167:U:H3    | 61:B2:294:C:HO2'   | 1.61                     | 0.47              |
| 61:B2:451:C:H5''  | 72:AE:57:ASN:HD22  | 1.80                     | 0.47              |
| 62:A5:577:A:N6    | 62:A5:579:A:N3     | 2.63                     | 0.47              |
| 62:A5:1041:A:H2'  | 62:A5:1042:G:H8    | 1.80                     | 0.47              |
| 62:A5:1470:C:H41  | 62:A5:1477:G:H5''  | 1.79                     | 0.47              |
| 62:A5:1536:U:H2'  | 62:A5:1537:G:C8    | 2.50                     | 0.47              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 62:A5:2744:C:H2'  | 62:A5:2745:A:H8    | 1.79                     | 0.47              |
| 62:A5:3178:G:H2'  | 62:A5:3179:A:H8    | 1.80                     | 0.47              |
| 62:A5:3341:C:H2'  | 62:A5:3342:C:H4'   | 1.97                     | 0.47              |
| 67:CU:264:LYS:HE3 | 67:CU:269:ARG:HE   | 1.79                     | 0.47              |
| 80:CM:5:ARG:NH1   | 80:CM:57:LEU:H     | 2.12                     | 0.47              |
| 10:AX:6:GLY:O     | 10:AX:9:THR:OG1    | 2.30                     | 0.46              |
| 10:AX:137:LYS:NZ  | 61:B2:31:C:O2'     | 2.48                     | 0.46              |
| 17:AP:84:ARG:HH12 | 17:AP:101:ASN:HA   | 1.80                     | 0.46              |
| 24:Ae:93:LYS:HG2  | 61:B2:594:G:H5''   | 1.97                     | 0.46              |
| 28:CN:71:ARG:NH2  | 62:A5:36:U:O3'     | 2.44                     | 0.46              |
| 29:CI:207:ALA:O   | 29:CI:211:LYS:N    | 2.41                     | 0.46              |
| 30:CD:202:GLN:HA  | 30:CD:205:ALA:HB3  | 1.97                     | 0.46              |
| 48:Cl:8:ARG:HH22  | 83:Cj:20:ARG:CZ    | 2.28                     | 0.46              |
| 51:Cp:51:VAL:HG12 | 51:Cp:52:VAL:H     | 1.80                     | 0.46              |
| 59:A8:111:G:HO2'  | 62:A5:1773:U:HO2'  | 1.62                     | 0.46              |
| 60:Cz:35:GLN:HE22 | 60:Cz:213:PRO:HB3  | 1.80                     | 0.46              |
| 61:B2:218:A:H5''  | 61:B2:917:U:H1'    | 1.95                     | 0.46              |
| 61:B2:1184:U:H3   | 64:AW:71:LYS:NZ    | 2.12                     | 0.46              |
| 62:A5:459:U:N3    | 62:A5:762:G:N7     | 2.60                     | 0.46              |
| 62:A5:1103:U:H2'  | 62:A5:1104:A:C8    | 2.50                     | 0.46              |
| 62:A5:1423:C:H1'  | 62:A5:3649:C:H42   | 1.81                     | 0.46              |
| 62:A5:1691:A:H61  | 62:A5:2733:G:H1'   | 1.80                     | 0.46              |
| 62:A5:1708:G:H22  | 62:A5:1753:G:H5'   | 1.80                     | 0.46              |
| 62:A5:1987:G:H5'' | 67:CU:253:ARG:HH22 | 1.80                     | 0.46              |
| 62:A5:2112:A:H2'  | 62:A5:2113:A:C8    | 2.50                     | 0.46              |
| 62:A5:2536:G:N2   | 62:A5:2555:G:O2'   | 2.48                     | 0.46              |
| 62:A5:2844:G:O6   | 62:A5:2845:G:N2    | 2.48                     | 0.46              |
| 62:A5:3122:A:H2'  | 62:A5:3123:G:H8    | 1.80                     | 0.46              |
| 62:A5:3585:A:N6   | 62:A5:3629:U:O2'   | 2.48                     | 0.46              |
| 62:A5:3890:G:C4   | 62:A5:3892:A:H5'   | 2.50                     | 0.46              |
| 78:CL:90:ALA:HA   | 78:CL:93:ILE:HD12  | 1.97                     | 0.46              |
| 78:CL:147:THR:OG1 | 78:CL:148:GLN:N    | 2.47                     | 0.46              |
| 78:CL:191:LEU:O   | 78:CL:195:ARG:N    | 2.45                     | 0.46              |
| 80:CM:126:ALA:O   | 80:CM:129:THR:OG1  | 2.28                     | 0.46              |
| 2:CA:162:ASN:OD1  | 2:CA:162:ASN:N     | 2.48                     | 0.46              |
| 4:CB:17:TYR:OH    | 62:A5:3582:A:OP1   | 2.34                     | 0.46              |
| 4:CB:47:ILE:H     | 4:CB:84:MET:HE1    | 1.79                     | 0.46              |
| 6:CC:36:ARG:NH2   | 31:CQ:22:ASP:OD2   | 2.31                     | 0.46              |
| 7:Ag:213:LYS:HG2  | 7:Ag:236:ILE:HG23  | 1.97                     | 0.46              |
| 19:AY:17:ARG:HD3  | 19:AY:20:ALA:HA    | 1.96                     | 0.46              |
| 23:AD:11:ARG:HA   | 23:AD:14:VAL:HG12  | 1.97                     | 0.46              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 23:AD:73:ALA:O     | 23:AD:77:LYS:NZ   | 2.41                     | 0.46              |
| 27:Ca:78:LYS:O     | 27:Ca:80:TRP:N    | 2.47                     | 0.46              |
| 34:CT:4:SER:OG     | 62:A5:3173:U:OP2  | 2.25                     | 0.46              |
| 34:CT:58:HIS:HE1   | 62:A5:1206:G:H5'  | 1.80                     | 0.46              |
| 36:CX:234:VAL:HG12 | 36:CX:240:ILE:HB  | 1.96                     | 0.46              |
| 53:CJ:25:LEU:HA    | 53:CJ:137:VAL:HA  | 1.98                     | 0.46              |
| 54:CH:86:PHE:N     | 54:CH:146:GLY:O   | 2.48                     | 0.46              |
| 59:A8:33:U:C6      | 83:Cj:74:PHE:CG   | 2.85                     | 0.46              |
| 61:B2:411:U:H2'    | 61:B2:412:A:C8    | 2.50                     | 0.46              |
| 61:B2:1043:U:O2    | 61:B2:1134:G:O2'  | 2.32                     | 0.46              |
| 61:B2:1444:C:H3'   | 69:AT:129:ARG:CZ  | 2.45                     | 0.46              |
| 61:B2:1693:C:P     | 69:AT:102:LYS:HE3 | 2.54                     | 0.46              |
| 62:A5:581:U:H2'    | 62:A5:582:A:H8    | 1.80                     | 0.46              |
| 62:A5:1180:U:C4    | 62:A5:1195:U:H1'  | 2.50                     | 0.46              |
| 62:A5:1811:A:H2'   | 62:A5:1812:C:H2'  | 1.97                     | 0.46              |
| 3:AB:29:ASP:HB2    | 3:AB:31:TYR:HE1   | 1.81                     | 0.46              |
| 10:AX:119:ARG:HH22 | 61:B2:1222:C:H5'' | 1.80                     | 0.46              |
| 12:AS:51:ASP:HB2   | 12:AS:54:LYS:HG3  | 1.97                     | 0.46              |
| 13:Ad:17:GLY:HA2   | 13:Ad:18:SER:HA   | 1.56                     | 0.46              |
| 27:Ca:59:MET:H     | 31:CQ:172:ARG:CZ  | 2.28                     | 0.46              |
| 29:CI:185:ARG:HA   | 29:CI:190:LEU:HB2 | 1.97                     | 0.46              |
| 30:CD:274:THR:HG23 | 30:CD:276:GLU:HG3 | 1.96                     | 0.46              |
| 35:CP:69:ARG:NH1   | 62:A5:2767:U:O2   | 2.31                     | 0.46              |
| 36:CX:221:THR:OG1  | 36:CX:222:HIS:N   | 2.46                     | 0.46              |
| 37:CY:50:ARG:HH12  | 37:CY:109:LEU:HB3 | 1.81                     | 0.46              |
| 37:CY:88:GLU:HA    | 37:CY:94:ASN:HA   | 1.97                     | 0.46              |
| 38:CZ:21:ARG:HD3   | 38:CZ:47:ASP:HA   | 1.96                     | 0.46              |
| 38:CZ:122:LYS:HA   | 38:CZ:122:LYS:HD2 | 1.72                     | 0.46              |
| 48:Cl:8:ARG:NH1    | 59:A8:109:U:OP1   | 2.48                     | 0.46              |
| 55:CE:130:PHE:HA   | 55:CE:135:CYS:H   | 1.80                     | 0.46              |
| 60:Cz:32:VAL:HA    | 60:Cz:208:SER:HA  | 1.97                     | 0.46              |
| 60:Cz:174:MET:SD   | 60:Cz:174:MET:N   | 2.82                     | 0.46              |
| 61:B2:142:A:N6     | 61:B2:166:A:OP2   | 2.48                     | 0.46              |
| 61:B2:189:C:H41    | 75:AI:145:GLU:HG2 | 1.81                     | 0.46              |
| 61:B2:1067:G:N2    | 61:B2:1109:C:N3   | 2.63                     | 0.46              |
| 61:B2:1173:A:H2'   | 61:B2:1174:A:C8   | 2.50                     | 0.46              |
| 62:A5:1458:G:N3    | 62:A5:1485:A:O2'  | 2.48                     | 0.46              |
| 62:A5:1893:C:H2'   | 62:A5:1894:G:H8   | 1.81                     | 0.46              |
| 62:A5:2997:C:OP1   | 66:Cg:102:LYS:NZ  | 2.46                     | 0.46              |
| 69:AT:69:PRO:HD2   | 69:AT:69:PRO:O    | 2.14                     | 0.46              |
| 72:AE:162:VAL:HG12 | 72:AE:169:ILE:HA  | 1.97                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 73:AG:58:LYS:HA    | 73:AG:59:GLN:HA    | 1.59                     | 0.46              |
| 74:AH:22:ILE:O     | 74:AH:26:LEU:N     | 2.48                     | 0.46              |
| 78:CL:57:VAL:H     | 78:CL:72:GLY:HA2   | 1.80                     | 0.46              |
| 3:AB:221:LEU:HD12  | 3:AB:222:LYS:HG2   | 1.97                     | 0.46              |
| 4:CB:117:ARG:HA    | 4:CB:177:LYS:HE2   | 1.97                     | 0.46              |
| 6:CC:291:ASP:OD1   | 6:CC:294:ARG:N     | 2.46                     | 0.46              |
| 7:Ag:256:SER:HA    | 7:Ag:272:ARG:HA    | 1.98                     | 0.46              |
| 9:AO:84:LYS:HA     | 9:AO:87:THR:HG23   | 1.97                     | 0.46              |
| 16:AR:15:VAL:O     | 16:AR:19:LYS:N     | 2.42                     | 0.46              |
| 19:AY:63:THR:HG23  | 19:AY:67:GLY:HA2   | 1.97                     | 0.46              |
| 30:CD:221:ARG:HH22 | 58:A7:31:G:H5'     | 1.80                     | 0.46              |
| 34:CT:78:LYS:HE2   | 34:CT:87:LYS:HG3   | 1.97                     | 0.46              |
| 38:CZ:107:LYS:NZ   | 62:A5:1946:G:OP1   | 2.41                     | 0.46              |
| 39:Cr:79:LYS:HA    | 39:Cr:79:LYS:HD2   | 1.61                     | 0.46              |
| 40:Ch:59:ILE:O     | 40:Ch:63:GLN:N     | 2.48                     | 0.46              |
| 42:Cc:61:GLU:OE1   | 42:Cc:61:GLU:N     | 2.46                     | 0.46              |
| 48:Cl:25:GLN:HA    | 48:Cl:28:ARG:HH22  | 1.80                     | 0.46              |
| 61:B2:1332:G:H5'   | 61:B2:1334:U:H5    | 1.80                     | 0.46              |
| 61:B2:1435:A:H61   | 61:B2:1570:U:H3    | 1.63                     | 0.46              |
| 61:B2:1727:U:N1    | 70:AF:190:ILE:CB   | 2.71                     | 0.46              |
| 62:A5:789:G:N7     | 62:A5:790:U:N3     | 2.64                     | 0.46              |
| 62:A5:3141:A:H2'   | 62:A5:3142:G:H8    | 1.79                     | 0.46              |
| 62:A5:3306:U:OP1   | 78:CL:190:ARG:NH2  | 2.48                     | 0.46              |
| 64:AW:30:CYS:H     | 64:AW:61:ILE:HD11  | 1.80                     | 0.46              |
| 70:AF:112:MET:HA   | 70:AF:115:ARG:HB3  | 1.98                     | 0.46              |
| 70:AF:192:THR:N    | 70:AF:195:GLU:OE2  | 2.47                     | 0.46              |
| 72:AE:41:SER:HA    | 72:AE:85:GLY:HA2   | 1.97                     | 0.46              |
| 72:AE:182:MET:HB3  | 72:AE:226:PHE:HB3  | 1.97                     | 0.46              |
| 75:AI:98:LYS:O     | 75:AI:100:SER:N    | 2.49                     | 0.46              |
| 1:AA:181:GLU:HA    | 1:AA:184:ARG:HB2   | 1.98                     | 0.46              |
| 4:CB:48:GLY:HA2    | 4:CB:81:THR:HB     | 1.97                     | 0.46              |
| 14:AN:4:MET:HE2    | 14:AN:4:MET:HB3    | 1.82                     | 0.46              |
| 14:AN:30:ALA:HB2   | 14:AN:66:VAL:HG22  | 1.98                     | 0.46              |
| 26:AJ:45:TRP:O     | 26:AJ:49:TYR:N     | 2.40                     | 0.46              |
| 27:Ca:74:ILE:HB    | 27:Ca:109:TYR:HB3  | 1.98                     | 0.46              |
| 30:CD:179:ARG:NE   | 62:A5:3278:A:OP1   | 2.48                     | 0.46              |
| 32:CR:136:ARG:HA   | 62:A5:2471:A:C8    | 2.51                     | 0.46              |
| 34:CT:11:THR:HB    | 34:CT:15:PHE:HB2   | 1.97                     | 0.46              |
| 35:CP:175:LEU:HA   | 35:CP:178:GLN:HE21 | 1.79                     | 0.46              |
| 36:CX:197:ILE:HD13 | 36:CX:229:HIS:HB3  | 1.98                     | 0.46              |
| 43:Cd:80:ARG:NH2   | 62:A5:3899:A:OP2   | 2.46                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 47:Ck:32:THR:HB    | 47:Ck:47:VAL:HG13  | 1.98                     | 0.46              |
| 53:CJ:144:TYR:OH   | 53:CJ:160:HIS:O    | 2.27                     | 0.46              |
| 54:CH:109:VAL:HG23 | 54:CH:110:ILE:H    | 1.81                     | 0.46              |
| 62:A5:178:U:O4     | 62:A5:271:A:N6     | 2.48                     | 0.46              |
| 62:A5:663:U:H3     | 62:A5:751:A:H5'    | 1.80                     | 0.46              |
| 62:A5:805:C:N4     | 62:A5:1681:G:O6    | 2.49                     | 0.46              |
| 62:A5:2701:G:O2'   | 62:A5:2703:G:OP2   | 2.27                     | 0.46              |
| 62:A5:2744:C:H2'   | 62:A5:2745:A:C8    | 2.50                     | 0.46              |
| 62:A5:3896:G:H22   | 62:A5:3959:U:H3    | 1.64                     | 0.46              |
| 69:AT:129:ARG:CB   | 69:AT:133:ARG:NE   | 2.78                     | 0.46              |
| 69:AT:138:ILE:O    | 69:AT:142:GLN:HG3  | 2.16                     | 0.46              |
| 71:CF:154:ARG:NH2  | 71:CF:192:GLU:OE2  | 2.45                     | 0.46              |
| 73:AG:187:GLN:HG3  | 73:AG:191:ARG:HH22 | 1.81                     | 0.46              |
| 75:AI:36:THR:OG1   | 75:AI:57:ALA:O     | 2.33                     | 0.46              |
| 78:CL:114:GLN:O    | 78:CL:118:GLU:N    | 2.47                     | 0.46              |
| 80:CM:34:ASN:OD1   | 80:CM:34:ASN:N     | 2.45                     | 0.46              |
| 1:AA:37:TYR:OH     | 18:AV:66:ASP:OD2   | 2.32                     | 0.46              |
| 1:AA:82:ILE:HD11   | 1:AA:168:ALA:HB2   | 1.97                     | 0.46              |
| 3:AB:54:GLY:HA3    | 62:A5:2818:G:H4'   | 1.96                     | 0.46              |
| 4:CB:390:GLY:O     | 4:CB:396:ARG:NE    | 2.48                     | 0.46              |
| 5:AC:53:VAL:HG12   | 5:AC:58:ILE:HB     | 1.96                     | 0.46              |
| 10:AX:8:ARG:N      | 61:B2:641:U:OP1    | 2.47                     | 0.46              |
| 10:AX:110:HIS:NE2  | 61:B2:1224:U:O4    | 2.47                     | 0.46              |
| 12:AS:14:ARG:HH11  | 12:AS:19:ASN:HB2   | 1.80                     | 0.46              |
| 14:AN:33:VAL:HA    | 14:AN:36:GLN:HB2   | 1.96                     | 0.46              |
| 19:AY:114:ARG:HD3  | 19:AY:128:THR:HG21 | 1.96                     | 0.46              |
| 22:Ab:42:ARG:HA    | 22:Ab:42:ARG:HD2   | 1.69                     | 0.46              |
| 29:CI:91:LEU:HD22  | 29:CI:135:ILE:HD12 | 1.98                     | 0.46              |
| 30:CD:245:GLN:O    | 30:CD:249:ASN:N    | 2.49                     | 0.46              |
| 32:CR:184:LEU:O    | 32:CR:188:HIS:N    | 2.48                     | 0.46              |
| 34:CT:4:SER:HA     | 34:CT:9:ARG:HD3    | 1.98                     | 0.46              |
| 55:CE:174:LYS:HD3  | 55:CE:178:LYS:HD3  | 1.98                     | 0.46              |
| 61:B2:388:G:H2'    | 61:B2:389:G:H8     | 1.80                     | 0.46              |
| 61:B2:1776:G:H1'   | 61:B2:1777:U:H5    | 1.80                     | 0.46              |
| 62:A5:237:G:N2     | 62:A5:247:C:O2     | 2.44                     | 0.46              |
| 62:A5:1035:G:O2'   | 62:A5:1056:G:N1    | 2.48                     | 0.46              |
| 62:A5:1475:A:O2'   | 62:A5:1494:C:O2    | 2.33                     | 0.46              |
| 62:A5:1982:U:OP1   | 66:Cg:1:MET:N      | 2.48                     | 0.46              |
| 62:A5:2160:C:C2    | 83:Cj:8:PHE:O      | 2.68                     | 0.46              |
| 62:A5:2848:A:O2'   | 62:A5:2883:C:O2'   | 2.31                     | 0.46              |
| 71:CF:231:TYR:HA   | 71:CF:235:GLY:HA2  | 1.97                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 76:AQ:125:ASP:N    | 76:AQ:125:ASP:OD1  | 2.48                     | 0.46              |
| 78:CL:33:ARG:O     | 78:CL:37:ASN:N     | 2.48                     | 0.46              |
| 1:AA:134:ILE:HG13  | 1:AA:144:VAL:HG21  | 1.96                     | 0.46              |
| 2:CA:67:TYR:HE1    | 62:A5:2919:A:H62   | 1.62                     | 0.46              |
| 2:CA:98:ILE:HA     | 2:CA:99:GLY:HA2    | 1.70                     | 0.46              |
| 2:CA:107:MET:O     | 2:CA:139:HIS:NE2   | 2.37                     | 0.46              |
| 5:AC:125:LYS:HE2   | 5:AC:125:LYS:HB3   | 1.67                     | 0.46              |
| 6:CC:376:LYS:HD2   | 6:CC:379:ALA:HB3   | 1.98                     | 0.46              |
| 11:AM:54:ALA:O     | 11:AM:80:GLN:NE2   | 2.48                     | 0.46              |
| 15:AL:102:ARG:NH2  | 61:B2:313:C:OP1    | 2.35                     | 0.46              |
| 27:Ca:65:ARG:NH2   | 62:A5:322:G:H21    | 2.13                     | 0.46              |
| 28:CN:143:ARG:HG2  | 40:Ch:95:LEU:HD22  | 1.96                     | 0.46              |
| 30:CD:265:LYS:HA   | 30:CD:266:LYS:HA   | 1.72                     | 0.46              |
| 36:CX:220:LEU:HD12 | 36:CX:220:LEU:HA   | 1.81                     | 0.46              |
| 39:Cr:57:PRO:HA    | 39:Cr:58:ALA:HA    | 1.63                     | 0.46              |
| 42:Cc:106:ARG:HA   | 42:Cc:106:ARG:HD2  | 1.69                     | 0.46              |
| 46:Ci:102:ASN:HA   | 46:Ci:105:THR:HG22 | 1.97                     | 0.46              |
| 48:Cl:8:ARG:NH2    | 83:Cj:20:ARG:CZ    | 2.76                     | 0.46              |
| 54:CH:134:ASN:HA   | 54:CH:142:LEU:HD13 | 1.97                     | 0.46              |
| 57:A9:24:G:O2'     | 62:A5:2:U:O2       | 2.34                     | 0.46              |
| 61:B2:248:G:H22    | 61:B2:254:C:H2'    | 1.80                     | 0.46              |
| 61:B2:279:G:H22    | 61:B2:287:C:H2'    | 1.80                     | 0.46              |
| 62:A5:1103:U:H2'   | 62:A5:1104:A:H8    | 1.81                     | 0.46              |
| 62:A5:3360:G:N1    | 62:A5:3361:U:O2    | 2.49                     | 0.46              |
| 66:Cg:49:GLU:OE2   | 66:Cg:50:LYS:N     | 2.48                     | 0.46              |
| 67:CU:264:LYS:HA   | 67:CU:267:SER:HA   | 1.97                     | 0.46              |
| 69:AT:50:PRO:CA    | 69:AT:53:PHE:CD2   | 2.90                     | 0.46              |
| 70:AF:122:GLU:O    | 70:AF:126:LEU:N    | 2.46                     | 0.46              |
| 72:AE:182:MET:HB2  | 72:AE:228:ILE:HD13 | 1.97                     | 0.46              |
| 75:AI:142:LYS:HA   | 75:AI:148:MET:HG3  | 1.98                     | 0.46              |
| 1:AA:176:TRP:HZ2   | 1:AA:201:LEU:HB2   | 1.81                     | 0.46              |
| 3:AB:210:LEU:HD21  | 3:AB:213:VAL:HG11  | 1.97                     | 0.46              |
| 7:Ag:20:GLN:HB3    | 7:Ag:70:VAL:HG12   | 1.98                     | 0.46              |
| 14:AN:83:ASP:HB3   | 14:AN:84:ILE:HD12  | 1.98                     | 0.46              |
| 15:AL:17:LEU:HD12  | 75:AI:194:GLY:HA3  | 1.98                     | 0.46              |
| 21:Aa:83:VAL:HG12  | 21:Aa:84:VAL:HG23  | 1.98                     | 0.46              |
| 26:AJ:144:ASN:H    | 61:B2:849:U:H5     | 1.63                     | 0.46              |
| 26:AJ:170:ARG:HB3  | 26:AJ:173:ARG:HB2  | 1.97                     | 0.46              |
| 37:CY:122:ARG:NE   | 62:A5:200:U:OP1    | 2.46                     | 0.46              |
| 38:CZ:10:ILE:HD11  | 38:CZ:87:ALA:HB2   | 1.97                     | 0.46              |
| 40:Ch:21:LEU:HD11  | 40:Ch:58:TYR:HE1   | 1.79                     | 0.46              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 45:Cf:49:ARG:CZ   | 55:CE:232:LEU:H    | 2.28                     | 0.46              |
| 53:CJ:62:VAL:HG13 | 53:CJ:64:SER:H     | 1.81                     | 0.46              |
| 56:CG:252:LEU:HA  | 56:CG:255:ILE:HB   | 1.96                     | 0.46              |
| 58:A7:69:C:H2'    | 58:A7:70:G:C8      | 2.51                     | 0.46              |
| 61:B2:608:U:H2'   | 61:B2:609:A:H8     | 1.81                     | 0.46              |
| 61:B2:1205:U:N3   | 61:B2:1206:G:N7    | 2.63                     | 0.46              |
| 61:B2:1820:U:O2   | 61:B2:1821:G:N2    | 2.48                     | 0.46              |
| 62:A5:63:G:H22    | 62:A5:348:A:H61    | 1.64                     | 0.46              |
| 62:A5:368:C:N4    | 62:A5:385:A:N7     | 2.63                     | 0.46              |
| 62:A5:1733:A:H3'  | 62:A5:1734:G:H8    | 1.81                     | 0.46              |
| 69:AT:16:LYS:HE2  | 69:AT:52:TRP:CH2   | 2.51                     | 0.46              |
| 76:AQ:49:LEU:HD13 | 76:AQ:87:ARG:HH12  | 1.81                     | 0.46              |
| 4:CB:53:MET:HG2   | 4:CB:77:THR:HG22   | 1.98                     | 0.46              |
| 7:Ag:40:LEU:HB3   | 7:Ag:60:LEU:HD23   | 1.97                     | 0.46              |
| 14:AN:78:VAL:HG23 | 14:AN:80:LEU:HD23  | 1.98                     | 0.46              |
| 18:AV:1:MET:HE1   | 18:AV:8:PHE:HA     | 1.98                     | 0.46              |
| 21:Aa:34:LYS:NZ   | 61:B2:1988:G:O6    | 2.42                     | 0.46              |
| 23:AD:125:LEU:HA  | 23:AD:128:ILE:HD11 | 1.97                     | 0.46              |
| 46:Ci:24:LYS:HE3  | 46:Ci:28:ASP:H     | 1.81                     | 0.46              |
| 52:Co:96:LYS:NZ   | 62:A5:3189:A:OP1   | 2.39                     | 0.46              |
| 55:CE:197:GLN:O   | 55:CE:201:ASP:N    | 2.41                     | 0.46              |
| 61:B2:122:G:OP1   | 72:AE:75:LYS:NZ    | 2.48                     | 0.46              |
| 61:B2:140:G:H5''  | 73:AG:143:LYS:HD2  | 1.98                     | 0.46              |
| 61:B2:1079:A:H3'  | 61:B2:1080:A:H8    | 1.81                     | 0.46              |
| 61:B2:1304:G:H1'  | 61:B2:1305:A:C8    | 2.51                     | 0.46              |
| 62:A5:2065:A:N7   | 62:A5:2066:G:N2    | 2.63                     | 0.46              |
| 62:A5:2654:G:H22  | 62:A5:2689:G:H1'   | 1.81                     | 0.46              |
| 62:A5:3256:U:OP2  | 62:A5:3260:G:N2    | 2.49                     | 0.46              |
| 63:Ac:24:THR:N    | 63:Ac:42:VAL:O     | 2.42                     | 0.46              |
| 69:AT:17:ALA:CA   | 69:AT:21:PHE:HE2   | 2.29                     | 0.46              |
| 73:AG:18:VAL:HG21 | 73:AG:41:LEU:HD11  | 1.98                     | 0.46              |
| 81:B:57:A:O2'     | 81:B:59:A:OP2      | 2.31                     | 0.46              |
| 2:CA:59:ALA:HB3   | 2:CA:76:PHE:HB2    | 1.98                     | 0.46              |
| 7:Ag:94:ALA:HA    | 7:Ag:95:ALA:HA     | 1.71                     | 0.46              |
| 29:CI:116:ARG:HA  | 29:CI:117:GLY:HA2  | 1.72                     | 0.46              |
| 29:CI:170:LYS:HA  | 29:CI:177:GLU:HA   | 1.98                     | 0.46              |
| 36:CX:159:ARG:N   | 62:A5:6:U:OP2      | 2.47                     | 0.46              |
| 45:Cf:39:VAL:HG22 | 45:Cf:41:ALA:H     | 1.81                     | 0.46              |
| 45:Cf:43:LYS:HZ1  | 45:Cf:45:LYS:HD2   | 1.81                     | 0.46              |
| 46:Ci:23:VAL:HG11 | 46:Ci:34:LEU:HB2   | 1.97                     | 0.46              |
| 47:Ck:1:MET:HE3   | 62:A5:2061:G:H5'   | 1.97                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 55:CE:216:HIS:ND1 | 55:CE:217:PRO:O   | 2.40                     | 0.46              |
| 56:CG:39:LYS:HD2  | 62:A5:3007:G:H1'  | 1.98                     | 0.46              |
| 56:CG:117:LEU:HA  | 56:CG:120:LYS:HG2 | 1.98                     | 0.46              |
| 61:B2:187:A:OP2   | 61:B2:196:G:N1    | 2.35                     | 0.46              |
| 61:B2:1025:G:H22  | 61:B2:1027:A:H3'  | 1.81                     | 0.46              |
| 61:B2:1295:U:H3   | 61:B2:1648:C:H5   | 1.62                     | 0.46              |
| 61:B2:1757:G:P    | 69:AT:38:LYS:HZ2  | 2.39                     | 0.46              |
| 61:B2:1947:U:H2'  | 61:B2:1948:A:H8   | 1.80                     | 0.46              |
| 61:B2:1970:U:O4   | 61:B2:1971:A:N6   | 2.49                     | 0.46              |
| 62:A5:1017:A:H4'  | 83:Cj:13:ASN:ND2  | 2.30                     | 0.46              |
| 62:A5:1429:U:N3   | 62:A5:1507:C:O2   | 2.47                     | 0.46              |
| 62:A5:2486:A:H2   | 62:A5:3918:A:H8   | 1.64                     | 0.46              |
| 62:A5:3906:U:O2   | 62:A5:3946:G:N2   | 2.49                     | 0.46              |
| 63:Ac:11:MET:HE3  | 63:Ac:11:MET:HB2  | 1.79                     | 0.46              |
| 69:AT:55:VAL:CG1  | 69:AT:55:VAL:O    | 2.64                     | 0.46              |
| 69:AT:129:ARG:HB3 | 69:AT:133:ARG:NE  | 2.31                     | 0.46              |
| 70:AF:57:ILE:HD12 | 70:AF:58:SER:HA   | 1.98                     | 0.46              |
| 72:AE:87:MET:SD   | 72:AE:100:ARG:NH2 | 2.89                     | 0.46              |
| 74:AH:35:LEU:HG   | 74:AH:39:LEU:HD22 | 1.98                     | 0.46              |
| 79:CV:118:THR:O   | 79:CV:118:THR:OG1 | 2.34                     | 0.46              |
| 80:CM:15:ALA:HB3  | 80:CM:20:LEU:HB2  | 1.97                     | 0.46              |
| 3:AB:27:ARG:O     | 3:AB:51:ARG:N     | 2.49                     | 0.45              |
| 3:AB:33:VAL:HA    | 3:AB:99:VAL:HG22  | 1.98                     | 0.45              |
| 5:AC:153:TRP:CZ2  | 5:AC:183:ARG:HG3  | 2.51                     | 0.45              |
| 7:Ag:32:ILE:HA    | 7:Ag:42:VAL:HA    | 1.99                     | 0.45              |
| 8:AU:32:ARG:O     | 8:AU:36:ASN:N     | 2.49                     | 0.45              |
| 10:AX:45:SER:OG   | 10:AX:46:HIS:N    | 2.49                     | 0.45              |
| 10:AX:132:ALA:HB1 | 10:AX:137:LYS:HB2 | 1.98                     | 0.45              |
| 15:AL:95:LYS:HB3  | 15:AL:96:TYR:CE2  | 2.51                     | 0.45              |
| 28:CN:81:TYR:HD1  | 62:A5:3141:A:H4'  | 1.80                     | 0.45              |
| 28:CN:155:VAL:O   | 28:CN:162:ARG:NH2 | 2.50                     | 0.45              |
| 35:CP:151:THR:OG1 | 35:CP:152:GLU:N   | 2.49                     | 0.45              |
| 46:Ci:95:ARG:CZ   | 62:A5:317:G:H5''  | 2.46                     | 0.45              |
| 61:B2:815:G:OP1   | 61:B2:817:C:N4    | 2.48                     | 0.45              |
| 61:B2:984:G:H1    | 61:B2:1003:C:H42  | 1.64                     | 0.45              |
| 61:B2:1540:G:OP1  | 69:AT:7:LYS:NZ    | 2.47                     | 0.45              |
| 62:A5:51:U:N3     | 62:A5:52:A:N7     | 2.63                     | 0.45              |
| 62:A5:953:U:H5''  | 62:A5:954:A:H5'   | 1.98                     | 0.45              |
| 62:A5:1751:U:H2'  | 62:A5:1752:G:C8   | 2.52                     | 0.45              |
| 62:A5:1951:C:H2'  | 62:A5:1952:A:H8   | 1.82                     | 0.45              |
| 62:A5:3717:U:O2'  | 62:A5:3719:A:N1   | 2.45                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 62:A5:3894:C:H2'   | 62:A5:3895:A:C8    | 2.51                     | 0.45              |
| 73:AG:74:ARG:HA    | 73:AG:96:SER:HA    | 1.98                     | 0.45              |
| 74:AH:152:VAL:HG13 | 74:AH:183:VAL:HG23 | 1.98                     | 0.45              |
| 74:AH:158:LYS:HD2  | 74:AH:158:LYS:HA   | 1.82                     | 0.45              |
| 78:CL:120:ARG:HD2  | 78:CL:123:LEU:HD23 | 1.98                     | 0.45              |
| 80:CM:145:LYS:O    | 80:CM:149:GLU:N    | 2.49                     | 0.45              |
| 14:AN:118:VAL:HA   | 14:AN:121:ARG:HB2  | 1.98                     | 0.45              |
| 23:AD:118:ARG:HH11 | 24:Ae:123:ARG:HG2  | 1.81                     | 0.45              |
| 27:Ca:13:ARG:HA    | 27:Ca:14:GLY:HA2   | 1.69                     | 0.45              |
| 28:CN:35:LYS:HA    | 28:CN:65:ARG:HE    | 1.82                     | 0.45              |
| 28:CN:81:TYR:CD1   | 62:A5:3141:A:H4'   | 2.51                     | 0.45              |
| 40:Ch:43:LYS:HZ2   | 40:Ch:45:SER:HA    | 1.80                     | 0.45              |
| 48:Cl:22:SER:OG    | 62:A5:1760:A:OP1   | 2.32                     | 0.45              |
| 54:CH:147:ASN:OD1  | 54:CH:147:ASN:N    | 2.43                     | 0.45              |
| 55:CE:35:LYS:HE2   | 55:CE:39:TYR:HB2   | 1.97                     | 0.45              |
| 58:A7:84:U:N3      | 62:A5:1412:A:N7    | 2.64                     | 0.45              |
| 60:Cz:179:LEU:HD12 | 60:Cz:182:ASN:HB3  | 1.99                     | 0.45              |
| 61:B2:588:A:O2'    | 61:B2:590:U:OP2    | 2.34                     | 0.45              |
| 61:B2:1079:A:C8    | 61:B2:1972:G:H1'   | 2.52                     | 0.45              |
| 61:B2:1288:G:OP2   | 61:B2:1787:U:O2'   | 2.34                     | 0.45              |
| 61:B2:1378:C:H42   | 61:B2:1410:C:H42   | 1.65                     | 0.45              |
| 62:A5:406:G:H2'    | 62:A5:407:A:C8     | 2.51                     | 0.45              |
| 62:A5:583:U:H3'    | 62:A5:584:A:C8     | 2.52                     | 0.45              |
| 62:A5:774:A:O2'    | 62:A5:777:C:OP2    | 2.33                     | 0.45              |
| 62:A5:865:A:O2'    | 62:A5:919:G:O2'    | 2.31                     | 0.45              |
| 62:A5:2533:U:H2'   | 62:A5:2534:G:C8    | 2.52                     | 0.45              |
| 62:A5:2624:G:H2'   | 62:A5:2625:G:C8    | 2.43                     | 0.45              |
| 62:A5:2798:C:N4    | 62:A5:2799:U:O4    | 2.49                     | 0.45              |
| 62:A5:2921:G:H2'   | 62:A5:2922:G:C8    | 2.52                     | 0.45              |
| 67:CU:238:LYS:HG3  | 67:CU:240:PHE:HB2  | 1.97                     | 0.45              |
| 69:AT:19:ALA:O     | 69:AT:23:LYS:CD    | 2.65                     | 0.45              |
| 69:AT:59:SER:HB2   | 69:AT:63:HIS:HE2   | 1.78                     | 0.45              |
| 73:AG:44:GLU:HA    | 73:AG:119:LYS:HE2  | 1.99                     | 0.45              |
| 80:CM:5:ARG:HH22   | 80:CM:56:HIS:HA    | 1.81                     | 0.45              |
| 8:AU:33:SER:HA     | 8:AU:36:ASN:HB2    | 1.99                     | 0.45              |
| 11:AM:71:LEU:HD22  | 25:Af:106:TYR:HB3  | 1.99                     | 0.45              |
| 28:CN:178:TYR:OH   | 62:A5:105:A:O4'    | 2.33                     | 0.45              |
| 29:CI:47:PRO:O     | 29:CI:178:ARG:NH2  | 2.45                     | 0.45              |
| 29:CI:170:LYS:O    | 29:CI:178:ARG:NH2  | 2.47                     | 0.45              |
| 30:CD:207:TYR:HE2  | 30:CD:222:GLN:HE21 | 1.64                     | 0.45              |
| 32:CR:124:TYR:O    | 32:CR:128:LYS:N    | 2.44                     | 0.45              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 39:Cr:55:VAL:HA   | 39:Cr:67:VAL:HG22  | 1.99                     | 0.45              |
| 54:CH:61:THR:OG1  | 54:CH:62:LYS:N     | 2.50                     | 0.45              |
| 56:CG:158:GLN:HB2 | 56:CG:209:LEU:HD23 | 1.98                     | 0.45              |
| 61:B2:58:U:H3     | 61:B2:88:G:H1      | 1.65                     | 0.45              |
| 61:B2:1457:C:H5'' | 61:B2:1458:U:H2'   | 1.99                     | 0.45              |
| 61:B2:1970:U:H2'  | 61:B2:1971:A:H8    | 1.81                     | 0.45              |
| 62:A5:107:G:HO2'  | 62:A5:849:U:HO2'   | 1.65                     | 0.45              |
| 62:A5:165:G:H22   | 62:A5:283:A:N6     | 2.15                     | 0.45              |
| 62:A5:1221:U:H2'  | 62:A5:1222:A:C8    | 2.51                     | 0.45              |
| 66:Cg:46:GLN:O    | 66:Cg:48:LYS:NZ    | 2.49                     | 0.45              |
| 67:CU:199:CYS:HA  | 67:CU:241:SER:HA   | 1.98                     | 0.45              |
| 69:AT:6:VAL:CB    | 69:AT:136:ASN:OD1  | 2.63                     | 0.45              |
| 7:Ag:258:LYS:HE2  | 7:Ag:260:TRP:HE1   | 1.82                     | 0.45              |
| 11:AM:65:GLU:OE2  | 61:B2:1315:U:N3    | 2.42                     | 0.45              |
| 14:AN:42:LYS:HG2  | 14:AN:80:LEU:HD11  | 1.97                     | 0.45              |
| 28:CN:36:LEU:HD12 | 28:CN:62:TYR:HD2   | 1.81                     | 0.45              |
| 32:CR:70:ARG:C    | 32:CR:73:GLY:H     | 2.24                     | 0.45              |
| 41:Cb:73:PRO:HB3  | 62:A5:1293:A:C6    | 2.51                     | 0.45              |
| 46:Ci:40:LYS:HE2  | 46:Ci:40:LYS:HB3   | 1.75                     | 0.45              |
| 47:Ck:24:LYS:N    | 47:Ck:35:LYS:O     | 2.38                     | 0.45              |
| 62:A5:34:C:H42    | 62:A5:59:G:H1      | 1.64                     | 0.45              |
| 62:A5:577:A:H1'   | 62:A5:635:G:N2     | 2.31                     | 0.45              |
| 62:A5:942:A:O2'   | 62:A5:944:G:OP1    | 2.29                     | 0.45              |
| 62:A5:1175:C:H2'  | 62:A5:1176:A:C8    | 2.51                     | 0.45              |
| 70:AF:85:PHE:O    | 70:AF:86:ARG:NE    | 2.44                     | 0.45              |
| 74:AH:15:PRO:HA   | 74:AH:16:ASP:HA    | 1.69                     | 0.45              |
| 80:CM:17:ALA:HB3  | 80:CM:54:ASN:HB3   | 1.98                     | 0.45              |
| 81:B:12:G:H1      | 81:B:22:C:H42      | 1.64                     | 0.45              |
| 4:CB:292:HIS:HB3  | 4:CB:293:THR:HG23  | 1.98                     | 0.45              |
| 10:AX:60:LYS:N    | 10:AX:114:ASP:O    | 2.47                     | 0.45              |
| 12:AS:134:GLN:NE2 | 61:B2:1736:U:OP1   | 2.50                     | 0.45              |
| 16:AR:96:ILE:HB   | 16:AR:117:LEU:HD13 | 1.99                     | 0.45              |
| 30:CD:215:ASP:HB2 | 30:CD:218:SER:HB3  | 1.99                     | 0.45              |
| 37:CY:44:VAL:HG11 | 37:CY:122:ARG:HB3  | 1.98                     | 0.45              |
| 38:CZ:51:ARG:HB2  | 38:CZ:65:LYS:HG3   | 1.98                     | 0.45              |
| 46:Ci:86:ARG:HD3  | 46:Ci:86:ARG:HA    | 1.77                     | 0.45              |
| 51:Cp:91:GLU:HG2  | 51:Cp:92:GLN:HG3   | 1.99                     | 0.45              |
| 61:B2:1445:A:C3'  | 69:AT:133:ARG:HH12 | 2.29                     | 0.45              |
| 61:B2:1924:C:O2'  | 75:AI:2:GLY:O      | 2.27                     | 0.45              |
| 62:A5:472:A:N7    | 62:A5:524:A:N6     | 2.57                     | 0.45              |
| 62:A5:805:C:O2    | 62:A5:1682:G:N2    | 2.49                     | 0.45              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 62:A5:2559:C:H2'  | 62:A5:2560:A:H8    | 1.81                     | 0.45              |
| 70:AF:146:ARG:HA  | 70:AF:170:ARG:HH11 | 1.81                     | 0.45              |
| 72:AE:139:LEU:N   | 72:AE:147:ILE:O    | 2.48                     | 0.45              |
| 72:AE:194:THR:O   | 72:AE:194:THR:OG1  | 2.33                     | 0.45              |
| 74:AH:17:ASP:N    | 74:AH:17:ASP:OD1   | 2.48                     | 0.45              |
| 74:AH:163:THR:O   | 74:AH:166:HIS:NE2  | 2.50                     | 0.45              |
| 75:AI:151:TYR:HE1 | 75:AI:154:ARG:HH11 | 1.64                     | 0.45              |
| 77:CO:194:PHE:HE2 | 77:CO:198:ILE:HD13 | 1.82                     | 0.45              |
| 80:CM:28:VAL:HG21 | 80:CM:47:ARG:HD3   | 1.98                     | 0.45              |
| 1:AA:167:SER:O    | 1:AA:170:SER:OG    | 2.29                     | 0.45              |
| 6:CC:319:LEU:HD21 | 62:A5:752:U:H5     | 1.81                     | 0.45              |
| 13:Ad:16:GLN:HE21 | 13:Ad:16:GLN:HB3   | 1.56                     | 0.45              |
| 18:AV:27:LYS:O    | 18:AV:29:HIS:ND1   | 2.41                     | 0.45              |
| 21:Aa:10:ARG:HB2  | 21:Aa:33:ASP:HB2   | 1.98                     | 0.45              |
| 26:AJ:19:ARG:NH2  | 61:B2:3:U:O2'      | 2.49                     | 0.45              |
| 30:CD:94:ASN:O    | 30:CD:98:ALA:N     | 2.50                     | 0.45              |
| 30:CD:182:GLY:HA3 | 30:CD:194:VAL:HG11 | 1.98                     | 0.45              |
| 39:Cr:79:LYS:HE3  | 39:Cr:82:VAL:HG22  | 1.99                     | 0.45              |
| 44:Ce:14:LYS:NZ   | 62:A5:1553:C:O2'   | 2.44                     | 0.45              |
| 44:Ce:30:LEU:HD11 | 62:A5:1674:A:C8    | 2.51                     | 0.45              |
| 49:Cm:102:ARG:O   | 62:A5:3654:C:N4    | 2.50                     | 0.45              |
| 54:CH:48:PRO:HB3  | 54:CH:54:LYS:HD2   | 1.99                     | 0.45              |
| 54:CH:105:GLU:OE1 | 54:CH:108:THR:OG1  | 2.34                     | 0.45              |
| 55:CE:59:LYS:HD2  | 55:CE:63:LYS:HA    | 1.98                     | 0.45              |
| 61:B2:279:G:N2    | 61:B2:288:C:O4'    | 2.49                     | 0.45              |
| 61:B2:355:G:N2    | 61:B2:1058:A:O2'   | 2.50                     | 0.45              |
| 61:B2:1053:A:H2'  | 61:B2:1054:A:H8    | 1.81                     | 0.45              |
| 62:A5:303:G:O2'   | 62:A5:304:U:H5''   | 2.16                     | 0.45              |
| 62:A5:843:A:H2'   | 62:A5:844:C:H6     | 1.81                     | 0.45              |
| 62:A5:906:A:H2'   | 62:A5:907:A:C8     | 2.51                     | 0.45              |
| 62:A5:1110:G:H1   | 62:A5:1118:C:H42   | 1.63                     | 0.45              |
| 62:A5:1809:A:H4'  | 62:A5:1810:A:C6    | 2.51                     | 0.45              |
| 62:A5:3188:A:H61  | 62:A5:3245:U:H3    | 1.62                     | 0.45              |
| 62:A5:3638:U:H2'  | 62:A5:3662:G:H22   | 1.81                     | 0.45              |
| 64:AW:39:THR:O    | 64:AW:43:LYS:N     | 2.49                     | 0.45              |
| 68:AK:51:HIS:HE1  | 68:AK:57:LYS:HA    | 1.82                     | 0.45              |
| 76:AQ:135:GLY:O   | 76:AQ:143:TYR:N    | 2.47                     | 0.45              |
| 78:CL:6:ASN:OD1   | 78:CL:6:ASN:N      | 2.50                     | 0.45              |
| 78:CL:143:CYS:HB2 | 78:CL:148:GLN:H    | 1.80                     | 0.45              |
| 4:CB:261:ARG:HB3  | 77:CO:66:VAL:HG11  | 1.99                     | 0.45              |
| 14:AN:46:THR:HG23 | 14:AN:49:LYS:H     | 1.81                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 14:AN:64:ARG:NH2   | 61:B2:1048:U:OP2   | 2.40                     | 0.45              |
| 16:AR:86:PRO:HA    | 16:AR:87:ALA:HA    | 1.58                     | 0.45              |
| 17:AP:89:VAL:HG13  | 17:AP:92:MET:H     | 1.80                     | 0.45              |
| 26:AJ:51:LEU:O     | 26:AJ:55:ARG:N     | 2.47                     | 0.45              |
| 28:CN:202:ARG:HD3  | 78:CL:27:GLN:HB3   | 1.98                     | 0.45              |
| 30:CD:211:LEU:HD23 | 30:CD:214:GLU:HB2  | 1.99                     | 0.45              |
| 32:CR:136:ARG:HA   | 62:A5:2471:A:H8    | 1.81                     | 0.45              |
| 33:CS:158:VAL:HG23 | 33:CS:160:HIS:H    | 1.81                     | 0.45              |
| 39:Cr:75:GLN:HG3   | 39:Cr:77:PRO:HA    | 1.99                     | 0.45              |
| 54:CH:110:ILE:HG12 | 54:CH:112:ILE:HG23 | 1.99                     | 0.45              |
| 61:B2:387:C:OP2    | 72:AE:10:LYS:NZ    | 2.39                     | 0.45              |
| 61:B2:457:G:OP2    | 61:B2:458:C:N4     | 2.47                     | 0.45              |
| 62:A5:191:A:N6     | 62:A5:260:A:N1     | 2.64                     | 0.45              |
| 62:A5:1026:G:OP1   | 62:A5:1874:G:O2'   | 2.35                     | 0.45              |
| 62:A5:1274:A:H2'   | 62:A5:1275:A:C8    | 2.51                     | 0.45              |
| 62:A5:1460:A:N6    | 62:A5:1486:A:N3    | 2.65                     | 0.45              |
| 62:A5:2161:G:H2'   | 83:Cj:5:THR:HG23   | 1.98                     | 0.45              |
| 62:A5:3857:G:H2'   | 62:A5:3858:A:C8    | 2.52                     | 0.45              |
| 64:AW:113:HIS:O    | 64:AW:117:ARG:N    | 2.45                     | 0.45              |
| 66:Cg:25:THR:HG23  | 66:Cg:30:LEU:H     | 1.81                     | 0.45              |
| 71:CF:97:ARG:HH12  | 71:CF:101:ILE:HD12 | 1.82                     | 0.45              |
| 75:AI:113:TYR:HB3  | 75:AI:117:TYR:HD2  | 1.81                     | 0.45              |
| 77:CO:175:GLU:O    | 77:CO:179:LEU:N    | 2.49                     | 0.45              |
| 2:CA:129:THR:HG23  | 62:A5:2555:G:H3'   | 1.99                     | 0.45              |
| 6:CC:339:LYS:HA    | 6:CC:339:LYS:HD3   | 1.77                     | 0.45              |
| 10:AX:133:LEU:HB3  | 10:AX:140:ARG:HH11 | 1.82                     | 0.45              |
| 12:AS:35:GLY:N     | 61:B2:1759:U:OP1   | 2.45                     | 0.45              |
| 15:AL:74:VAL:HG21  | 15:AL:83:ILE:HD12  | 1.99                     | 0.45              |
| 17:AP:120:GLY:HA2  | 17:AP:123:ALA:HB3  | 1.99                     | 0.45              |
| 24:Ae:90:LYS:HD2   | 24:Ae:90:LYS:HA    | 1.73                     | 0.45              |
| 28:CN:31:ARG:HD3   | 28:CN:31:ARG:HA    | 1.65                     | 0.45              |
| 28:CN:151:ILE:HD11 | 28:CN:159:ARG:HD3  | 1.99                     | 0.45              |
| 31:CQ:8:LYS:NZ     | 62:A5:1170:U:OP1   | 2.49                     | 0.45              |
| 37:CY:14:ASN:HD21  | 62:A5:236:G:N2     | 2.15                     | 0.45              |
| 38:CZ:67:LYS:HD2   | 38:CZ:114:ARG:HH21 | 1.81                     | 0.45              |
| 49:Cm:109:ASN:OD1  | 49:Cm:109:ASN:N    | 2.50                     | 0.45              |
| 51:Cp:3:LYS:HA     | 51:Cp:3:LYS:HD2    | 1.76                     | 0.45              |
| 53:CJ:45:LEU:HD22  | 53:CJ:53:PRO:HB3   | 1.98                     | 0.45              |
| 53:CJ:95:ARG:NH1   | 53:CJ:113:GLY:O    | 2.41                     | 0.45              |
| 54:CH:90:MET:HB2   | 54:CH:142:LEU:HB2  | 1.98                     | 0.45              |
| 58:A7:17:C:H2'     | 58:A7:18:G:C8      | 2.52                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 58:A7:70:G:H2'     | 58:A7:71:G:H8      | 1.82                     | 0.45              |
| 59:A8:92:G:OP2     | 83:Cj:76:ASN:ND2   | 2.49                     | 0.45              |
| 59:A8:108:A:C6     | 83:Cj:29:LEU:CD1   | 3.00                     | 0.45              |
| 61:B2:72:A:N7      | 73:AG:168:LYS:NZ   | 2.65                     | 0.45              |
| 61:B2:489:C:H2'    | 61:B2:490:A:C8     | 2.52                     | 0.45              |
| 61:B2:504:A:H2'    | 61:B2:505:G:H8     | 1.82                     | 0.45              |
| 61:B2:1778:A:H62   | 61:B2:1802:G:H21   | 1.65                     | 0.45              |
| 62:A5:173:A:H2'    | 62:A5:174:A:C8     | 2.52                     | 0.45              |
| 62:A5:795:A:H1'    | 62:A5:797:A:C8     | 2.52                     | 0.45              |
| 62:A5:848:A:O3'    | 78:CL:68:LYS:NZ    | 2.49                     | 0.45              |
| 62:A5:2904:U:H2'   | 62:A5:2905:A:C8    | 2.51                     | 0.45              |
| 69:AT:30:VAL:HG12  | 69:AT:31:PRO:CD    | 2.47                     | 0.45              |
| 69:AT:122:LYS:NZ   | 69:AT:128:GLN:NE2  | 2.65                     | 0.45              |
| 72:AE:51:ARG:HB3   | 72:AE:111:ILE:HD11 | 1.99                     | 0.45              |
| 76:AQ:112:ASP:N    | 76:AQ:112:ASP:OD1  | 2.50                     | 0.45              |
| 78:CL:132:LYS:HE3  | 78:CL:132:LYS:HB3  | 1.78                     | 0.45              |
| 2:CA:188:LYS:HE3   | 2:CA:192:LYS:HD2   | 1.98                     | 0.45              |
| 3:AB:114:ARG:NH1   | 61:B2:1017:A:O2'   | 2.49                     | 0.45              |
| 4:CB:16:PHE:HB2    | 4:CB:17:TYR:CD2    | 2.52                     | 0.45              |
| 4:CB:101:ALA:O     | 62:A5:3680:A:O2'   | 2.32                     | 0.45              |
| 8:AU:69:LYS:HB3    | 8:AU:80:ASP:HB2    | 1.99                     | 0.45              |
| 14:AN:151:ALA:HB1  | 42:Cc:84:ALA:HA    | 1.98                     | 0.45              |
| 21:Aa:92:ARG:NH2   | 61:B2:1990:U:OP2   | 2.39                     | 0.45              |
| 26:AJ:177:LYS:HE2  | 61:B2:544:C:H5'    | 1.99                     | 0.45              |
| 28:CN:83:LYS:HD3   | 28:CN:85:LYS:NZ    | 2.32                     | 0.45              |
| 30:CD:166:ALA:HB1  | 30:CD:171:LEU:HD12 | 1.98                     | 0.45              |
| 31:CQ:137:LEU:HD23 | 31:CQ:137:LEU:HA   | 1.86                     | 0.45              |
| 32:CR:84:THR:OG1   | 62:A5:1033:U:OP1   | 2.25                     | 0.45              |
| 48:Cl:2:ALA:HB2    | 62:A5:1735:G:N7    | 2.32                     | 0.45              |
| 54:CH:44:ASP:O     | 54:CH:56:GLU:N     | 2.48                     | 0.45              |
| 61:B2:219:A:OP2    | 61:B2:917:U:O2'    | 2.32                     | 0.45              |
| 61:B2:1062:C:H2'   | 61:B2:1063:G:C8    | 2.50                     | 0.45              |
| 62:A5:120:C:H42    | 62:A5:282:A:H4'    | 1.82                     | 0.45              |
| 62:A5:702:A:N6     | 62:A5:703:A:N3     | 2.65                     | 0.45              |
| 62:A5:1575:U:H3    | 62:A5:1584:A:H61   | 1.64                     | 0.45              |
| 62:A5:2235:G:H21   | 62:A5:2249:A:H62   | 1.65                     | 0.45              |
| 62:A5:3477:A:H1'   | 62:A5:3512:U:C5    | 2.52                     | 0.45              |
| 69:AT:122:LYS:NZ   | 69:AT:128:GLN:HE22 | 2.15                     | 0.45              |
| 73:AG:165:LYS:H    | 73:AG:170:ALA:HB2  | 1.82                     | 0.45              |
| 78:CL:125:LEU:HG   | 78:CL:137:GLU:H    | 1.82                     | 0.45              |
| 1:AA:185:LEU:HD12  | 18:AV:46:GLN:HB2   | 1.99                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:CB:336:CYS:HB2   | 62:A5:3583:C:H1'   | 1.97                     | 0.45              |
| 19:AY:88:PRO:O     | 19:AY:92:LEU:N     | 2.46                     | 0.45              |
| 21:Aa:43:ASN:HA    | 21:Aa:66:LYS:HG2   | 1.97                     | 0.45              |
| 23:AD:30:GLU:HA    | 68:AK:59:GLN:HE22  | 1.82                     | 0.45              |
| 27:Ca:99:ALA:HA    | 27:Ca:100:PRO:HD3  | 1.78                     | 0.45              |
| 45:Cf:53:LYS:HD3   | 45:Cf:53:LYS:HA    | 1.79                     | 0.45              |
| 54:CH:76:GLU:HA    | 54:CH:79:ILE:HG12  | 1.98                     | 0.45              |
| 56:CG:229:THR:HA   | 56:CG:233:GLU:HB2  | 1.98                     | 0.45              |
| 59:A8:20:C:N4      | 59:A8:21:U:O4      | 2.49                     | 0.45              |
| 61:B2:1573:U:O2'   | 61:B2:1708:A:N1    | 2.42                     | 0.45              |
| 61:B2:1970:U:H2'   | 61:B2:1971:A:C8    | 2.52                     | 0.45              |
| 62:A5:137:U:O2     | 62:A5:140:A:N6     | 2.46                     | 0.45              |
| 62:A5:214:A:H1'    | 62:A5:240:G:C8     | 2.52                     | 0.45              |
| 62:A5:620:U:O2'    | 62:A5:622:A:N7     | 2.47                     | 0.45              |
| 62:A5:781:C:H2'    | 62:A5:782:G:C8     | 2.52                     | 0.45              |
| 62:A5:817:C:H2'    | 62:A5:818:A:C8     | 2.52                     | 0.45              |
| 62:A5:975:A:H2'    | 62:A5:976:A:C8     | 2.51                     | 0.45              |
| 62:A5:1577:A:C5    | 62:A5:1578:C:H1'   | 2.52                     | 0.45              |
| 62:A5:3208:A:N3    | 62:A5:3211:A:N6    | 2.63                     | 0.45              |
| 62:A5:3609:A:H61   | 62:A5:3612:A:N6    | 2.15                     | 0.45              |
| 69:AT:133:ARG:O    | 69:AT:137:GLN:HG3  | 2.15                     | 0.45              |
| 73:AG:20:ASP:OD2   | 73:AG:23:LYS:NZ    | 2.49                     | 0.45              |
| 74:AH:99:LEU:HD22  | 74:AH:112:GLN:HG3  | 1.99                     | 0.45              |
| 74:AH:108:ASN:OD1  | 74:AH:108:ASN:N    | 2.50                     | 0.45              |
| 74:AH:137:ILE:HD13 | 74:AH:154:VAL:HG13 | 1.99                     | 0.45              |
| 76:AQ:34:LEU:HD21  | 76:AQ:65:PHE:HB3   | 1.99                     | 0.45              |
| 2:CA:33:ASP:OD1    | 2:CA:33:ASP:N      | 2.41                     | 0.44              |
| 2:CA:188:LYS:NZ    | 62:A5:2106:C:O2    | 2.41                     | 0.44              |
| 4:CB:220:VAL:O     | 4:CB:346:THR:OG1   | 2.33                     | 0.44              |
| 16:AR:42:PRO:HG2   | 16:AR:46:LEU:HD12  | 1.98                     | 0.44              |
| 17:AP:84:ARG:O     | 17:AP:120:GLY:N    | 2.49                     | 0.44              |
| 18:AV:35:ASN:HA    | 18:AV:52:THR:HA    | 2.00                     | 0.44              |
| 28:CN:135:ILE:HD12 | 28:CN:151:ILE:HD13 | 1.98                     | 0.44              |
| 31:CQ:30:LYS:HD3   | 62:A5:1596:A:H5'   | 1.98                     | 0.44              |
| 31:CQ:92:LEU:HD23  | 31:CQ:95:VAL:HG12  | 1.99                     | 0.44              |
| 32:CR:19:LYS:N     | 62:A5:2191:G:OP1   | 2.41                     | 0.44              |
| 35:CP:57:CYS:HB3   | 35:CP:72:GLN:HB2   | 1.97                     | 0.44              |
| 36:CX:159:ARG:CZ   | 57:A9:24:G:H4'     | 2.47                     | 0.44              |
| 36:CX:163:THR:HG23 | 56:CG:56:LEU:HD13  | 1.99                     | 0.44              |
| 37:CY:121:ARG:NH2  | 62:A5:199:U:O5'    | 2.41                     | 0.44              |
| 40:Ch:70:ARG:HD3   | 62:A5:139:U:N3     | 2.32                     | 0.44              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 43:Cd:117:GLU:OE1  | 43:Cd:119:VAL:N   | 2.48                     | 0.44              |
| 46:Ci:101:SER:O    | 46:Ci:105:THR:N   | 2.46                     | 0.44              |
| 53:CJ:107:THR:HG23 | 53:CJ:109:ASN:H   | 1.81                     | 0.44              |
| 55:CE:184:ILE:HD12 | 55:CE:184:ILE:HA  | 1.86                     | 0.44              |
| 57:A9:24:G:H22     | 62:A5:3117:A:H8   | 1.64                     | 0.44              |
| 59:A8:86:A:H3'     | 59:A8:87:A:H8     | 1.82                     | 0.44              |
| 61:B2:151:G:H1     | 61:B2:157:C:H42   | 1.64                     | 0.44              |
| 61:B2:611:U:H2'    | 61:B2:612:A:H8    | 1.81                     | 0.44              |
| 61:B2:1670:G:P     | 69:AT:43:LYS:NZ   | 2.89                     | 0.44              |
| 62:A5:196:C:H2'    | 62:A5:197:G:C8    | 2.52                     | 0.44              |
| 62:A5:660:A:H2'    | 62:A5:661:G:C8    | 2.52                     | 0.44              |
| 62:A5:841:A:O2'    | 62:A5:842:A:OP1   | 2.34                     | 0.44              |
| 62:A5:939:A:N1     | 62:A5:962:U:N3    | 2.66                     | 0.44              |
| 62:A5:2503:G:H1    | 62:A5:2707:C:N4   | 2.14                     | 0.44              |
| 69:AT:71:GLY:O     | 69:AT:75:ILE:CG1  | 2.64                     | 0.44              |
| 71:CF:101:ILE:HD12 | 71:CF:101:ILE:HA  | 1.81                     | 0.44              |
| 2:CA:147:ARG:HG2   | 2:CA:157:VAL:HG22 | 1.97                     | 0.44              |
| 6:CC:124:ARG:HB2   | 6:CC:280:TYR:CZ   | 2.51                     | 0.44              |
| 6:CC:359:LYS:HE3   | 6:CC:359:LYS:HB3  | 1.83                     | 0.44              |
| 11:AM:64:ASP:OD1   | 11:AM:64:ASP:N    | 2.50                     | 0.44              |
| 15:AL:119:HIS:HA   | 15:AL:120:GLY:HA2 | 1.71                     | 0.44              |
| 19:AY:92:LEU:HD23  | 19:AY:96:GLY:HA2  | 2.00                     | 0.44              |
| 23:AD:34:ASP:O     | 23:AD:55:THR:OG1  | 2.35                     | 0.44              |
| 24:Ae:125:ARG:NH2  | 24:Ae:126:GLY:O   | 2.50                     | 0.44              |
| 27:Ca:52:GLY:N     | 31:CQ:178:ARG:O   | 2.49                     | 0.44              |
| 32:CR:184:LEU:HA   | 32:CR:187:LEU:HB2 | 1.98                     | 0.44              |
| 34:CT:17:ARG:HH22  | 34:CT:45:HIS:CE1  | 2.34                     | 0.44              |
| 46:Ci:11:LEU:HD22  | 78:CL:189:ALA:HB2 | 2.00                     | 0.44              |
| 61:B2:532:U:N3     | 61:B2:535:A:OP2   | 2.46                     | 0.44              |
| 61:B2:1164:G:H2'   | 61:B2:1165:C:C6   | 2.53                     | 0.44              |
| 61:B2:1565:C:OP1   | 76:AQ:6:ARG:NH2   | 2.40                     | 0.44              |
| 62:A5:56:A:H4'     | 83:Cj:48:ASN:HB2  | 1.99                     | 0.44              |
| 62:A5:173:A:H2'    | 62:A5:174:A:H8    | 1.82                     | 0.44              |
| 62:A5:619:U:O2'    | 62:A5:621:A:N6    | 2.49                     | 0.44              |
| 62:A5:2022:C:H2'   | 62:A5:2023:A:C8   | 2.52                     | 0.44              |
| 62:A5:2167:G:N1    | 62:A5:2168:G:O6   | 2.51                     | 0.44              |
| 70:AF:152:ILE:HA   | 70:AF:158:VAL:HA  | 1.99                     | 0.44              |
| 72:AE:19:MET:HE3   | 72:AE:51:ARG:HG3  | 1.98                     | 0.44              |
| 72:AE:186:GLY:H    | 72:AE:189:LEU:HB3 | 1.82                     | 0.44              |
| 73:AG:136:LYS:HE3  | 73:AG:136:LYS:HB3 | 1.61                     | 0.44              |
| 75:AI:143:ARG:HG3  | 75:AI:145:GLU:HB2 | 1.99                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 79:CV:19:GLY:HA2   | 79:CV:86:LYS:HE3   | 1.99                     | 0.44              |
| 2:CA:179:ILE:H     | 2:CA:179:ILE:HG13  | 1.61                     | 0.44              |
| 3:AB:125:GLU:O     | 3:AB:168:ARG:NH1   | 2.43                     | 0.44              |
| 4:CB:133:ALA:HA    | 4:CB:136:LYS:HD3   | 1.99                     | 0.44              |
| 6:CC:5:ASN:HB2     | 6:CC:8:PRO:HB3     | 1.98                     | 0.44              |
| 6:CC:150:VAL:HG13  | 39:Cr:79:LYS:HG3   | 1.99                     | 0.44              |
| 7:Ag:19:THR:HG22   | 7:Ag:288:LEU:HD23  | 2.00                     | 0.44              |
| 18:AV:50:SER:OG    | 18:AV:51:LYS:N     | 2.50                     | 0.44              |
| 20:AZ:104:SER:OG   | 70:AF:115:ARG:NH1  | 2.50                     | 0.44              |
| 23:AD:127:TYR:O    | 23:AD:131:SER:N    | 2.41                     | 0.44              |
| 25:Af:136:GLU:OE2  | 25:Af:138:ARG:NH2  | 2.51                     | 0.44              |
| 30:CD:282:ILE:O    | 30:CD:286:LYS:N    | 2.48                     | 0.44              |
| 32:CR:91:THR:OG1   | 32:CR:92:LYS:N     | 2.49                     | 0.44              |
| 34:CT:3:ASN:O      | 34:CT:9:ARG:NE     | 2.50                     | 0.44              |
| 34:CT:117:LYS:HD2  | 34:CT:120:LYS:HD2  | 1.99                     | 0.44              |
| 35:CP:178:GLN:HG3  | 35:CP:179:LYS:HE2  | 1.99                     | 0.44              |
| 39:Cr:30:SER:OG    | 39:Cr:35:ASN:OD1   | 2.35                     | 0.44              |
| 42:Cc:29:LEU:HD11  | 42:Cc:87:LYS:HE3   | 2.00                     | 0.44              |
| 45:Cf:81:LYS:HB2   | 45:Cf:124:ILE:HD12 | 1.99                     | 0.44              |
| 48:Cl:49:LEU:HD23  | 48:Cl:49:LEU:HA    | 1.74                     | 0.44              |
| 54:CH:162:SER:HA   | 54:CH:163:THR:HA   | 1.67                     | 0.44              |
| 55:CE:51:LYS:HA    | 55:CE:51:LYS:HD3   | 1.87                     | 0.44              |
| 56:CG:153:GLU:OE1  | 56:CG:154:GLN:NE2  | 2.50                     | 0.44              |
| 61:B2:225:G:H21    | 61:B2:238:C:H41    | 1.65                     | 0.44              |
| 61:B2:568:U:H2'    | 61:B2:569:G:C8     | 2.52                     | 0.44              |
| 61:B2:574:C:N4     | 61:B2:584:G:O2'    | 2.51                     | 0.44              |
| 61:B2:907:U:O2'    | 61:B2:938:G:O6     | 2.27                     | 0.44              |
| 61:B2:1122:A:O4'   | 64:AW:2:VAL:N      | 2.50                     | 0.44              |
| 61:B2:1727:U:C5    | 70:AF:190:ILE:HA   | 2.52                     | 0.44              |
| 62:A5:728:U:H2'    | 62:A5:729:G:C8     | 2.53                     | 0.44              |
| 62:A5:1259:A:O2'   | 62:A5:1261:A:OP2   | 2.32                     | 0.44              |
| 62:A5:1404:A:N3    | 77:CO:51:ARG:NH2   | 2.66                     | 0.44              |
| 62:A5:1684:G:H2'   | 62:A5:1685:G:H8    | 1.83                     | 0.44              |
| 62:A5:1987:G:C2    | 62:A5:1988:A:H1'   | 2.52                     | 0.44              |
| 62:A5:3461:C:H2'   | 62:A5:3462:A:H8    | 1.82                     | 0.44              |
| 62:A5:3849:A:H2'   | 62:A5:3850:A:C8    | 2.52                     | 0.44              |
| 67:CU:272:LEU:HD13 | 67:CU:286:TYR:HA   | 1.99                     | 0.44              |
| 72:AE:94:LYS:HA    | 72:AE:95:THR:HA    | 1.66                     | 0.44              |
| 75:AI:74:ARG:HA    | 75:AI:74:ARG:HD3   | 1.83                     | 0.44              |
| 81:B:11:C:H42      | 81:B:23:G:H1       | 1.66                     | 0.44              |
| 4:CB:70:LYS:HZ3    | 4:CB:71:GLU:N      | 2.15                     | 0.44              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 5:AC:162:THR:OG1   | 5:AC:163:VAL:N    | 2.51                     | 0.44              |
| 10:AX:7:LEU:HD12   | 15:AL:98:ARG:HG2  | 1.98                     | 0.44              |
| 20:AZ:62:PRO:HA    | 20:AZ:63:ALA:HA   | 1.65                     | 0.44              |
| 29:CI:88:ARG:N     | 29:CI:137:SER:O   | 2.43                     | 0.44              |
| 30:CD:53:VAL:O     | 30:CD:54:ARG:NH1  | 2.44                     | 0.44              |
| 38:CZ:92:PHE:HD2   | 38:CZ:116:LYS:HB2 | 1.82                     | 0.44              |
| 45:Cf:40:SER:O     | 62:A5:1396:A:N6   | 2.51                     | 0.44              |
| 55:CE:123:LEU:HD11 | 62:A5:3842:A:H5'  | 1.98                     | 0.44              |
| 56:CG:71:GLN:O     | 56:CG:75:LEU:N    | 2.45                     | 0.44              |
| 58:A7:29:C:H1'     | 58:A7:50:A:H61    | 1.82                     | 0.44              |
| 62:A5:194:A:H2'    | 62:A5:195:A:H8    | 1.81                     | 0.44              |
| 62:A5:1086:C:H2'   | 62:A5:1087:G:H8   | 1.82                     | 0.44              |
| 62:A5:1461:G:O2'   | 62:A5:1479:G:OP2  | 2.35                     | 0.44              |
| 62:A5:1978:G:H2'   | 62:A5:1979:A:C8   | 2.53                     | 0.44              |
| 62:A5:2162:C:H3'   | 62:A5:2163:A:H8   | 1.82                     | 0.44              |
| 62:A5:3594:A:O2'   | 62:A5:3947:C:O2'  | 2.27                     | 0.44              |
| 69:AT:6:VAL:HG21   | 69:AT:136:ASN:ND2 | 2.32                     | 0.44              |
| 69:AT:122:LYS:HZ3  | 69:AT:128:GLN:NE2 | 2.15                     | 0.44              |
| 71:CF:182:LEU:HD22 | 71:CF:186:HIS:HB2 | 1.99                     | 0.44              |
| 78:CL:125:LEU:HD12 | 78:CL:135:ALA:HB1 | 1.98                     | 0.44              |
| 80:CM:13:ALA:N     | 80:CM:25:VAL:O    | 2.43                     | 0.44              |
| 80:CM:148:ARG:HA   | 80:CM:148:ARG:HD3 | 1.82                     | 0.44              |
| 1:AA:122:LEU:HD23  | 1:AA:144:VAL:HG22 | 1.99                     | 0.44              |
| 5:AC:62:GLU:HG2    | 18:AV:12:TYR:HB3  | 1.99                     | 0.44              |
| 10:AX:51:VAL:HB    | 10:AX:97:ASN:H    | 1.83                     | 0.44              |
| 11:AM:93:GLY:HA2   | 11:AM:114:SER:HA  | 2.00                     | 0.44              |
| 35:CP:4:TYR:OH     | 35:CP:18:ARG:N    | 2.51                     | 0.44              |
| 38:CZ:113:THR:HA   | 38:CZ:116:LYS:HB3 | 2.00                     | 0.44              |
| 43:Cd:39:ALA:HB1   | 43:Cd:42:ALA:HB3  | 1.99                     | 0.44              |
| 45:Cf:121:VAL:HG13 | 45:Cf:133:ALA:HB2 | 1.99                     | 0.44              |
| 46:CI:78:ARG:O     | 46:CI:82:PHE:N    | 2.51                     | 0.44              |
| 54:CH:139:LYS:NZ   | 54:CH:140:ASP:OD2 | 2.39                     | 0.44              |
| 54:CH:173:PHE:HE1  | 62:A5:3560:C:H4'  | 1.81                     | 0.44              |
| 58:A7:30:G:H2'     | 58:A7:31:G:C8     | 2.53                     | 0.44              |
| 61:B2:334:G:H5''   | 75:AI:98:LYS:HD3  | 1.99                     | 0.44              |
| 61:B2:988:G:N2     | 61:B2:988:G:OP2   | 2.50                     | 0.44              |
| 61:B2:1783:U:P     | 69:AT:92:PHE:CE2  | 3.11                     | 0.44              |
| 62:A5:89:A:OP1     | 62:A5:104:A:N6    | 2.51                     | 0.44              |
| 62:A5:357:C:OP1    | 62:A5:1621:A:O2'  | 2.35                     | 0.44              |
| 62:A5:1292:G:O2'   | 62:A5:1294:U:OP2  | 2.36                     | 0.44              |
| 62:A5:1426:U:H2'   | 62:A5:1427:G:C8   | 2.51                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 62:A5:1881:C:H2'   | 62:A5:1882:G:C8    | 2.52                     | 0.44              |
| 62:A5:3788:G:C2    | 80:CM:150:ARG:HD2  | 2.52                     | 0.44              |
| 64:AW:17:ALA:HB1   | 64:AW:22:LYS:HB2   | 2.00                     | 0.44              |
| 67:CU:218:HIS:HA   | 67:CU:225:LEU:HD22 | 1.99                     | 0.44              |
| 67:CU:268:LEU:HD12 | 67:CU:268:LEU:HA   | 1.89                     | 0.44              |
| 75:AI:84:ASN:H     | 75:AI:91:VAL:HG22  | 1.81                     | 0.44              |
| 76:AQ:91:SER:HB3   | 76:AQ:121:LEU:HD12 | 2.00                     | 0.44              |
| 2:CA:5:ILE:HG23    | 2:CA:209:HIS:HA    | 2.00                     | 0.44              |
| 3:AB:108:LEU:HB3   | 3:AB:216:ARG:HG2   | 1.99                     | 0.44              |
| 5:AC:235:THR:HB    | 5:AC:238:LEU:HG    | 1.98                     | 0.44              |
| 6:CC:34:PRO:HB2    | 6:CC:36:ARG:HG3    | 1.99                     | 0.44              |
| 7:Ag:81:SER:O      | 7:Ag:81:SER:OG     | 2.36                     | 0.44              |
| 7:Ag:201:VAL:HG22  | 7:Ag:205:GLY:HA2   | 2.00                     | 0.44              |
| 9:AO:97:LEU:O      | 9:AO:132:VAL:N     | 2.45                     | 0.44              |
| 11:AM:37:GLY:H     | 11:AM:119:LYS:H    | 1.66                     | 0.44              |
| 12:AS:47:LYS:HA    | 12:AS:47:LYS:HD2   | 1.79                     | 0.44              |
| 12:AS:87:GLN:HA    | 12:AS:95:TYR:HA    | 1.99                     | 0.44              |
| 15:AL:18:ASN:HD21  | 61:B2:210:U:H4'    | 1.81                     | 0.44              |
| 19:AY:77:TYR:HE1   | 19:AY:86:PHE:HD2   | 1.66                     | 0.44              |
| 22:Ab:82:LYS:NZ    | 22:Ab:83:PRO:O     | 2.51                     | 0.44              |
| 26:AJ:30:LEU:O     | 26:AJ:34:GLY:N     | 2.49                     | 0.44              |
| 28:CN:165:THR:HG23 | 28:CN:168:GLY:H    | 1.82                     | 0.44              |
| 30:CD:72:ASP:OD2   | 58:A7:7:G:O2'      | 2.26                     | 0.44              |
| 30:CD:242:LYS:O    | 30:CD:245:GLN:NE2  | 2.51                     | 0.44              |
| 33:CS:11:GLU:HG3   | 33:CS:65:LYS:HB2   | 2.00                     | 0.44              |
| 35:CP:115:HIS:HB2  | 35:CP:151:THR:HG22 | 1.99                     | 0.44              |
| 37:CY:100:HIS:CE1  | 37:CY:102:SER:HB3  | 2.53                     | 0.44              |
| 38:CZ:135:PHE:HE2  | 66:Cg:85:LEU:HD11  | 1.81                     | 0.44              |
| 40:Ch:17:LEU:O     | 40:Ch:21:LEU:N     | 2.48                     | 0.44              |
| 58:A7:108:G:H2'    | 58:A7:109:U:H6     | 1.83                     | 0.44              |
| 61:B2:421:A:H5''   | 61:B2:422:A:N7     | 2.32                     | 0.44              |
| 62:A5:389:G:N2     | 62:A5:393:A:H62    | 2.16                     | 0.44              |
| 62:A5:1121:A:C2    | 83:Cj:8:PHE:HZ     | 2.32                     | 0.44              |
| 62:A5:1614:A:H2    | 62:A5:1615:G:C6    | 2.36                     | 0.44              |
| 62:A5:2258:U:H3    | 62:A5:2485:A:H61   | 1.64                     | 0.44              |
| 62:A5:3151:G:N3    | 62:A5:3351:A:H1'   | 2.32                     | 0.44              |
| 62:A5:3595:U:H4'   | 62:A5:3946:G:H21   | 1.82                     | 0.44              |
| 62:A5:3754:C:H5''  | 62:A5:3756:A:C6    | 2.53                     | 0.44              |
| 62:A5:3849:A:N1    | 62:A5:3850:A:N6    | 2.66                     | 0.44              |
| 63:Ac:38:ILE:HG12  | 63:Ac:40:ARG:HE    | 1.82                     | 0.44              |
| 68:AK:20:VAL:HG12  | 68:AK:68:TYR:HA    | 2.00                     | 0.44              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 73:AG:79:LYS:HA   | 73:AG:80:GLY:HA2   | 1.57                     | 0.44              |
| 74:AH:78:VAL:HG12 | 74:AH:90:VAL:HG23  | 2.00                     | 0.44              |
| 75:AI:142:LYS:HD2 | 75:AI:148:MET:HE2  | 2.00                     | 0.44              |
| 76:AQ:42:GLU:OE1  | 76:AQ:43:GLN:NE2   | 2.38                     | 0.44              |
| 76:AQ:125:ASP:HA  | 76:AQ:126:PRO:HD3  | 1.88                     | 0.44              |
| 77:CO:78:PRO:HD3  | 77:CO:149:TRP:CD2  | 2.53                     | 0.44              |
| 78:CL:195:ARG:HA  | 78:CL:198:ARG:HB2  | 1.99                     | 0.44              |
| 81:B:29:G:H2'     | 81:B:30:G:H8       | 1.82                     | 0.44              |
| 83:Cj:21:ARG:O    | 83:Cj:21:ARG:HD3   | 2.16                     | 0.44              |
| 1:AA:206:ASP:OD2  | 1:AA:211:GLU:N     | 2.51                     | 0.44              |
| 2:CA:139:HIS:HA   | 2:CA:146:THR:HG22  | 1.99                     | 0.44              |
| 2:CA:178:PRO:HG2  | 51:Cp:22:LEU:HD11  | 2.00                     | 0.44              |
| 4:CB:89:ALA:HA    | 4:CB:162:VAL:HA    | 2.00                     | 0.44              |
| 4:CB:140:ASP:HB2  | 4:CB:144:LYS:HE2   | 1.98                     | 0.44              |
| 5:AC:175:SER:O    | 5:AC:175:SER:OG    | 2.31                     | 0.44              |
| 16:AR:100:ALA:HB2 | 16:AR:118:GLN:HB2  | 1.99                     | 0.44              |
| 26:AJ:41:LYS:HD2  | 61:B2:600:A:H5''   | 1.99                     | 0.44              |
| 26:AJ:81:ARG:NH2  | 61:B2:844:A:OP1    | 2.47                     | 0.44              |
| 29:CI:98:ARG:NE   | 62:A5:1341:G:OP2   | 2.33                     | 0.44              |
| 29:CI:209:TRP:HZ3 | 30:CD:289:TYR:HD2  | 1.66                     | 0.44              |
| 36:CX:166:HIS:NE2 | 62:A5:2916:U:O3'   | 2.48                     | 0.44              |
| 38:CZ:53:VAL:HG22 | 38:CZ:65:LYS:HB3   | 2.00                     | 0.44              |
| 39:Cr:76:ARG:HD3  | 39:Cr:78:ALA:HB3   | 1.99                     | 0.44              |
| 56:CG:196:GLY:HA2 | 56:CG:199:VAL:HG22 | 1.99                     | 0.44              |
| 60:Cz:33:GLU:HB2  | 60:Cz:207:LYS:HE3  | 2.00                     | 0.44              |
| 60:Cz:206:VAL:O   | 60:Cz:214:GLN:N    | 2.50                     | 0.44              |
| 61:B2:153:A:H2'   | 61:B2:154:A:C8     | 2.53                     | 0.44              |
| 61:B2:353:U:H2'   | 61:B2:354:U:H6     | 1.82                     | 0.44              |
| 61:B2:1782:G:O3'  | 69:AT:92:PHE:CD2   | 2.63                     | 0.44              |
| 62:A5:169:C:N4    | 62:A5:170:G:O6     | 2.51                     | 0.44              |
| 62:A5:347:A:H5''  | 62:A5:347:A:C8     | 2.53                     | 0.44              |
| 62:A5:622:A:H2'   | 62:A5:623:C:H4'    | 1.99                     | 0.44              |
| 62:A5:712:U:H2'   | 62:A5:713:U:H6     | 1.82                     | 0.44              |
| 62:A5:1707:A:H3'  | 62:A5:1708:G:H8    | 1.83                     | 0.44              |
| 62:A5:2204:U:H2'  | 62:A5:2205:G:O4'   | 2.18                     | 0.44              |
| 62:A5:2847:G:N3   | 62:A5:2871:G:N2    | 2.66                     | 0.44              |
| 62:A5:3178:G:H2'  | 62:A5:3179:A:C8    | 2.53                     | 0.44              |
| 62:A5:3492:G:H2'  | 62:A5:3493:U:C6    | 2.53                     | 0.44              |
| 63:Ac:52:LEU:HD13 | 70:AF:167:PRO:HD3  | 1.99                     | 0.44              |
| 68:AK:51:HIS:CE1  | 68:AK:57:LYS:HA    | 2.53                     | 0.44              |
| 69:AT:29:LYS:HZ1  | 69:AT:108:GLU:C    | 2.24                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 78:CL:58:VAL:HA    | 78:CL:69:LEU:HB2   | 1.99                     | 0.44              |
| 80:CM:143:LEU:HD23 | 80:CM:143:LEU:HA   | 1.88                     | 0.44              |
| 83:Cj:21:ARG:HD3   | 83:Cj:21:ARG:C     | 2.43                     | 0.44              |
| 83:Cj:28:HIS:O     | 83:Cj:29:LEU:C     | 2.60                     | 0.44              |
| 4:CB:166:SER:O     | 4:CB:168:ILE:N     | 2.51                     | 0.44              |
| 6:CC:117:LYS:HE2   | 62:A5:832:U:C5     | 2.53                     | 0.44              |
| 7:Ag:62:GLY:O      | 61:B2:1426:A:O2'   | 2.35                     | 0.44              |
| 9:AO:122:SER:HB2   | 9:AO:124:MET:HE2   | 2.00                     | 0.44              |
| 11:AM:123:GLU:HA   | 11:AM:128:LEU:HD12 | 2.00                     | 0.44              |
| 16:AR:27:ASP:O     | 16:AR:31:ASN:ND2   | 2.51                     | 0.44              |
| 23:AD:107:LEU:O    | 23:AD:111:LEU:N    | 2.48                     | 0.44              |
| 27:Ca:74:ILE:HD11  | 27:Ca:82:LEU:HD11  | 2.00                     | 0.44              |
| 29:CI:144:TYR:HB3  | 29:CI:147:GLN:HB2  | 1.99                     | 0.44              |
| 30:CD:75:VAL:O     | 30:CD:112:LYS:NZ   | 2.51                     | 0.44              |
| 34:CT:21:LYS:HE2   | 34:CT:21:LYS:HB3   | 1.87                     | 0.44              |
| 42:Cc:40:GLN:HG3   | 42:Cc:42:LYS:H     | 1.83                     | 0.44              |
| 46:Ci:16:LYS:HZ3   | 78:CL:105:SER:HA   | 1.83                     | 0.44              |
| 49:Cm:104:HIS:CE1  | 62:A5:3653:U:H4'   | 2.53                     | 0.44              |
| 50:Cn:7:LYS:O      | 50:Cn:11:ARG:N     | 2.40                     | 0.44              |
| 55:CE:205:VAL:O    | 55:CE:209:LEU:N    | 2.50                     | 0.44              |
| 59:A8:105:C:C2     | 59:A8:106:A:H1'    | 2.52                     | 0.44              |
| 61:B2:936:G:H4'    | 61:B2:937:A:C5     | 2.53                     | 0.44              |
| 61:B2:1226:A:H2'   | 61:B2:1227:A:H8    | 1.83                     | 0.44              |
| 61:B2:1367:C:H2'   | 61:B2:1368:G:C8    | 2.53                     | 0.44              |
| 61:B2:1381:G:N2    | 61:B2:1409:A:O4'   | 2.44                     | 0.44              |
| 61:B2:1442:U:O2    | 61:B2:1543:G:N2    | 2.51                     | 0.44              |
| 61:B2:1600:A:N7    | 61:B2:1605:G:N2    | 2.66                     | 0.44              |
| 62:A5:474:A:N6     | 62:A5:524:A:O4'    | 2.50                     | 0.44              |
| 62:A5:2049:G:H2'   | 62:A5:2050:U:H6    | 1.83                     | 0.44              |
| 62:A5:2774:G:OP1   | 62:A5:2775:A:O2'   | 2.33                     | 0.44              |
| 62:A5:3261:U:H2'   | 62:A5:3262:A:C8    | 2.53                     | 0.44              |
| 62:A5:3448:U:O2'   | 79:CV:47:GLY:O     | 2.35                     | 0.44              |
| 62:A5:3773:G:H5'   | 62:A5:3779:U:H5    | 1.83                     | 0.44              |
| 64:AW:48:GLY:H     | 64:AW:65:LEU:HA    | 1.83                     | 0.44              |
| 64:AW:51:GLU:HG2   | 74:AH:143:ARG:HG2  | 1.99                     | 0.44              |
| 69:AT:63:HIS:ND1   | 69:AT:67:ARG:CZ    | 2.81                     | 0.44              |
| 74:AH:169:ASP:O    | 74:AH:172:THR:OG1  | 2.33                     | 0.44              |
| 77:CO:202:GLY:HA2  | 77:CO:205:VAL:HG22 | 2.00                     | 0.44              |
| 1:AA:63:ARG:NH1    | 18:AV:78:ILE:O     | 2.51                     | 0.44              |
| 5:AC:147:PRO:HB3   | 18:AV:11:LEU:HD23  | 1.99                     | 0.44              |
| 7:Ag:5:LEU:HD11    | 7:Ag:313:VAL:HG22  | 1.99                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:Ag:126:ARG:O     | 7:Ag:128:LYS:NZ    | 2.42                     | 0.44              |
| 15:AL:131:LEU:HD13 | 15:AL:135:VAL:HG12 | 1.99                     | 0.44              |
| 21:Aa:34:LYS:HE2   | 21:Aa:34:LYS:HB3   | 1.88                     | 0.44              |
| 26:AJ:47:VAL:HG13  | 26:AJ:103:ILE:HD11 | 2.00                     | 0.44              |
| 28:CN:195:LYS:HE2  | 28:CN:195:LYS:HB2  | 1.57                     | 0.44              |
| 30:CD:20:PHE:HB3   | 58:A7:10:C:C2      | 2.53                     | 0.44              |
| 33:CS:56:LYS:HA    | 33:CS:57:THR:HA    | 1.72                     | 0.44              |
| 34:CT:106:LEU:HD13 | 34:CT:106:LEU:HA   | 1.81                     | 0.44              |
| 44:Ce:66:ARG:NH1   | 62:A5:1645:G:O3'   | 2.51                     | 0.44              |
| 54:CH:35:LYS:HE3   | 54:CH:35:LYS:HB3   | 1.87                     | 0.44              |
| 59:A8:35:G:N2      | 59:A8:36:A:N1      | 2.65                     | 0.44              |
| 61:B2:178:A:H2'    | 61:B2:179:A:C8     | 2.52                     | 0.44              |
| 61:B2:366:C:H2'    | 61:B2:367:G:C8     | 2.53                     | 0.44              |
| 61:B2:492:G:H2'    | 61:B2:493:A:C8     | 2.52                     | 0.44              |
| 61:B2:660:G:OP1    | 61:B2:701:G:N2     | 2.51                     | 0.44              |
| 61:B2:950:U:H3'    | 64:AW:28:ARG:HH12  | 1.83                     | 0.44              |
| 61:B2:1344:A:C8    | 68:AK:4:PRO:HB3    | 2.53                     | 0.44              |
| 61:B2:1381:G:H2'   | 61:B2:1382:G:C8    | 2.53                     | 0.44              |
| 61:B2:1445:A:P     | 69:AT:129:ARG:CD   | 2.96                     | 0.44              |
| 61:B2:1581:A:P     | 61:B2:1603:G:H1    | 2.41                     | 0.44              |
| 61:B2:1716:A:OP1   | 69:AT:78:ILE:HG21  | 2.00                     | 0.44              |
| 62:A5:423:U:O4     | 62:A5:424:G:N2     | 2.51                     | 0.44              |
| 62:A5:1208:U:H2'   | 62:A5:1209:A:C8    | 2.52                     | 0.44              |
| 62:A5:1360:U:H5''  | 62:A5:1361:G:OP2   | 2.17                     | 0.44              |
| 62:A5:1465:A:N6    | 62:A5:1478:A:O2'   | 2.51                     | 0.44              |
| 62:A5:2160:C:O2    | 83:Cj:8:PHE:HB3    | 2.18                     | 0.44              |
| 62:A5:2166:U:H3'   | 62:A5:2167:G:H8    | 1.83                     | 0.44              |
| 62:A5:2660:U:OP1   | 62:A5:3504:G:O2'   | 2.26                     | 0.44              |
| 62:A5:3141:A:H2'   | 62:A5:3142:G:C8    | 2.53                     | 0.44              |
| 64:AW:53:VAL:HA    | 74:AH:141:ARG:HA   | 2.00                     | 0.44              |
| 69:AT:144:ASP:HA   | 69:AT:147:LYS:CE   | 2.48                     | 0.44              |
| 80:CM:9:THR:HA     | 80:CM:10:GLY:HA2   | 1.75                     | 0.44              |
| 80:CM:82:LEU:O     | 80:CM:86:TRP:N     | 2.51                     | 0.44              |
| 5:AC:151:GLY:O     | 5:AC:162:THR:N     | 2.43                     | 0.43              |
| 7:Ag:18:VAL:HG11   | 7:Ag:308:ILE:HG12  | 2.00                     | 0.43              |
| 9:AO:86:LYS:NZ     | 9:AO:124:MET:SD    | 2.75                     | 0.43              |
| 10:AX:60:LYS:H     | 10:AX:114:ASP:HB3  | 1.83                     | 0.43              |
| 10:AX:101:LEU:HB2  | 10:AX:124:LYS:HB2  | 2.00                     | 0.43              |
| 11:AM:90:LYS:HD2   | 11:AM:90:LYS:HA    | 1.84                     | 0.43              |
| 19:AY:10:THR:O     | 19:AY:10:THR:OG1   | 2.34                     | 0.43              |
| 19:AY:90:TYR:HB2   | 61:B2:450:A:H5'    | 1.99                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:Ab:7:LEU:HD23  | 64:AW:62:VAL:HG23  | 1.99                     | 0.43              |
| 23:AD:26:PHE:O    | 23:AD:30:GLU:N     | 2.49                     | 0.43              |
| 25:Af:138:ARG:NE  | 61:B2:1322:C:O2    | 2.50                     | 0.43              |
| 26:AJ:109:ARG:HA  | 26:AJ:114:GLN:HE21 | 1.82                     | 0.43              |
| 28:CN:23:LEU:O    | 28:CN:27:VAL:N     | 2.51                     | 0.43              |
| 32:CR:30:ASN:OD1  | 32:CR:30:ASN:N     | 2.46                     | 0.43              |
| 32:CR:84:THR:HA   | 62:A5:2231:A:H4'   | 1.99                     | 0.43              |
| 37:CY:12:ARG:NH2  | 59:A8:24:G:O6      | 2.51                     | 0.43              |
| 47:Ck:1:MET:HE1   | 47:Ck:35:LYS:HD3   | 2.00                     | 0.43              |
| 53:CJ:2:ALA:O     | 58:A7:61:G:O2'     | 2.28                     | 0.43              |
| 53:CJ:148:HIS:O   | 58:A7:43:U:O2'     | 2.29                     | 0.43              |
| 54:CH:46:TYR:HB3  | 80:CM:1:MET:H1     | 1.83                     | 0.43              |
| 54:CH:166:LYS:HD2 | 54:CH:166:LYS:HA   | 1.85                     | 0.43              |
| 61:B2:1350:G:C5   | 61:B2:1351:G:H1'   | 2.53                     | 0.43              |
| 62:A5:375:C:H42   | 62:A5:380:G:H1     | 1.65                     | 0.43              |
| 62:A5:2747:G:H2'  | 62:A5:2748:G:C8    | 2.53                     | 0.43              |
| 62:A5:3658:G:H2'  | 62:A5:3659:G:H8    | 1.82                     | 0.43              |
| 63:Ac:18:GLY:HA2  | 63:Ac:22:GLN:HA    | 2.00                     | 0.43              |
| 69:AT:40:ALA:HB2  | 69:AT:95:ALA:HA    | 2.00                     | 0.43              |
| 74:AH:101:LYS:HE2 | 74:AH:101:LYS:HB3  | 1.79                     | 0.43              |
| 74:AH:170:THR:O   | 74:AH:173:SER:OG   | 2.33                     | 0.43              |
| 75:AI:76:THR:HB   | 75:AI:108:PRO:HG3  | 1.99                     | 0.43              |
| 78:CL:112:ASN:O   | 78:CL:116:LEU:N    | 2.44                     | 0.43              |
| 1:AA:34:MET:HB2   | 1:AA:154:LEU:HD11  | 2.00                     | 0.43              |
| 4:CB:89:ALA:N     | 4:CB:104:ASN:OD1   | 2.50                     | 0.43              |
| 4:CB:235:TRP:HE1  | 4:CB:268:ARG:H     | 1.65                     | 0.43              |
| 4:CB:261:ARG:HH22 | 77:CO:70:ARG:NH1   | 2.15                     | 0.43              |
| 5:AC:234:LEU:HD23 | 18:AV:23:ILE:HD12  | 1.99                     | 0.43              |
| 6:CC:47:LEU:HD11  | 6:CC:123:ARG:HD3   | 2.00                     | 0.43              |
| 6:CC:333:PRO:HB2  | 71:CF:54:LEU:HD13  | 2.00                     | 0.43              |
| 10:AX:64:SER:O    | 10:AX:64:SER:OG    | 2.32                     | 0.43              |
| 18:AV:57:GLY:O    | 18:AV:61:ARG:N     | 2.51                     | 0.43              |
| 28:CN:46:ASP:O    | 28:CN:47:LYS:NZ    | 2.37                     | 0.43              |
| 29:CI:214:ARG:HA  | 29:CI:214:ARG:HD3  | 1.73                     | 0.43              |
| 32:CR:7:GLN:HG2   | 32:CR:32:ILE:HG22  | 2.00                     | 0.43              |
| 36:CX:162:ARG:HD2 | 36:CX:162:ARG:HA   | 1.76                     | 0.43              |
| 38:CZ:48:ARG:H    | 38:CZ:69:LYS:HB3   | 1.83                     | 0.43              |
| 39:Cr:80:ASN:HB2  | 39:Cr:82:VAL:HA    | 1.98                     | 0.43              |
| 43:Cd:51:GLU:O    | 43:Cd:55:GLY:N     | 2.47                     | 0.43              |
| 46:CI:24:LYS:HG2  | 46:CI:27:GLY:HA2   | 1.99                     | 0.43              |
| 48:Cl:48:LYS:HA   | 48:Cl:48:LYS:HD3   | 1.72                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 56:CG:111:SER:O   | 56:CG:115:LYS:N    | 2.40                     | 0.43              |
| 61:B2:149:U:O2    | 73:AG:4:ASN:ND2    | 2.51                     | 0.43              |
| 61:B2:644:A:H4'   | 64:AW:31:SER:HB2   | 2.00                     | 0.43              |
| 61:B2:844:A:HO2'  | 72:AE:255:ARG:HH12 | 1.61                     | 0.43              |
| 61:B2:904:C:H41   | 61:B2:938:G:N2     | 2.16                     | 0.43              |
| 61:B2:1252:G:O2'  | 61:B2:1804:U:O2    | 2.31                     | 0.43              |
| 61:B2:1661:A:H4'  | 61:B2:1733:G:H4'   | 2.01                     | 0.43              |
| 62:A5:508:U:H2'   | 62:A5:509:A:C8     | 2.54                     | 0.43              |
| 62:A5:557:G:N2    | 62:A5:655:C:N3     | 2.57                     | 0.43              |
| 62:A5:1447:C:OP2  | 62:A5:1479:G:N2    | 2.52                     | 0.43              |
| 62:A5:1772:G:N2   | 62:A5:2148:C:O2    | 2.51                     | 0.43              |
| 62:A5:1982:U:H2'  | 62:A5:1983:A:H8    | 1.83                     | 0.43              |
| 62:A5:2002:C:H2'  | 62:A5:2003:U:C6    | 2.52                     | 0.43              |
| 62:A5:3601:U:H2'  | 62:A5:3602:U:C6    | 2.53                     | 0.43              |
| 62:A5:3676:C:H3'  | 62:A5:3677:U:C5'   | 2.48                     | 0.43              |
| 65:CW:39:SER:OG   | 65:CW:44:ARG:NH1   | 2.47                     | 0.43              |
| 73:AG:5:VAL:HG13  | 73:AG:124:LEU:HD11 | 2.00                     | 0.43              |
| 74:AH:58:VAL:HB   | 74:AH:90:VAL:HG12  | 2.00                     | 0.43              |
| 80:CM:117:ARG:HG2 | 80:CM:121:LYS:HD2  | 2.01                     | 0.43              |
| 6:CC:83:ARG:HA    | 6:CC:83:ARG:HD2    | 1.81                     | 0.43              |
| 6:CC:177:LEU:HD23 | 6:CC:177:LEU:HA    | 1.75                     | 0.43              |
| 6:CC:264:ASN:OD1  | 6:CC:264:ASN:N     | 2.50                     | 0.43              |
| 9:AO:29:GLY:O     | 9:AO:94:HIS:N      | 2.48                     | 0.43              |
| 17:AP:103:LYS:HD2 | 17:AP:104:ASP:H    | 1.83                     | 0.43              |
| 18:AV:64:GLU:O    | 18:AV:68:SER:OG    | 2.32                     | 0.43              |
| 26:AJ:13:THR:HG22 | 26:AJ:14:TYR:H     | 1.84                     | 0.43              |
| 27:Ca:59:MET:SD   | 62:A5:3319:A:O2'   | 2.76                     | 0.43              |
| 34:CT:43:LYS:HE3  | 34:CT:43:LYS:HB2   | 1.74                     | 0.43              |
| 37:CY:29:LEU:HD23 | 37:CY:29:LEU:HA    | 1.80                     | 0.43              |
| 40:Ch:106:LYS:HD2 | 62:A5:116:U:H5'    | 1.99                     | 0.43              |
| 40:Ch:117:ARG:NH2 | 78:CL:126:PHE:O    | 2.34                     | 0.43              |
| 44:Ce:91:ASN:ND2  | 44:Ce:92:ARG:N     | 2.66                     | 0.43              |
| 46:Ci:18:SER:O    | 46:Ci:18:SER:OG    | 2.31                     | 0.43              |
| 61:B2:953:A:H2'   | 61:B2:954:A:C8     | 2.54                     | 0.43              |
| 61:B2:984:G:H22   | 61:B2:1003:C:H42   | 1.64                     | 0.43              |
| 61:B2:1346:C:H1'  | 68:AK:1:MET:HE1    | 2.01                     | 0.43              |
| 62:A5:43:A:H3'    | 62:A5:44:A:H4'     | 2.00                     | 0.43              |
| 62:A5:564:C:N4    | 62:A5:647:A:H61    | 2.13                     | 0.43              |
| 62:A5:709:U:H2'   | 62:A5:710:A:C8     | 2.48                     | 0.43              |
| 62:A5:753:U:H1'   | 62:A5:754:A:H8     | 1.84                     | 0.43              |
| 62:A5:867:U:H3'   | 62:A5:868:A:C8     | 2.53                     | 0.43              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 62:A5:930:U:H2'    | 62:A5:931:A:C8    | 2.53                     | 0.43              |
| 62:A5:1286:U:H3    | 62:A5:1299:A:H61  | 1.66                     | 0.43              |
| 62:A5:3618:A:H2'   | 62:A5:3619:U:C6   | 2.54                     | 0.43              |
| 71:CF:147:TYR:CZ   | 71:CF:241:GLU:HB2 | 2.53                     | 0.43              |
| 73:AG:121:ILE:HD12 | 73:AG:122:PRO:HD2 | 2.01                     | 0.43              |
| 76:AQ:18:LYS:HG3   | 76:AQ:19:LYS:HE2  | 2.00                     | 0.43              |
| 76:AQ:120:THR:OG1  | 76:AQ:123:VAL:O   | 2.36                     | 0.43              |
| 80:CM:145:LYS:HD2  | 80:CM:145:LYS:HA  | 1.80                     | 0.43              |
| 81:B:15:G:N2       | 81:B:19:A:H61     | 2.16                     | 0.43              |
| 7:Ag:108:ASP:HB3   | 7:Ag:126:ARG:HD2  | 1.99                     | 0.43              |
| 7:Ag:218:LEU:HD11  | 7:Ag:227:ASN:HB3  | 1.99                     | 0.43              |
| 11:AM:49:LEU:HB3   | 11:AM:54:ALA:HB2  | 1.99                     | 0.43              |
| 13:Ad:7:TRP:O      | 61:B2:1642:C:O2'  | 2.30                     | 0.43              |
| 19:AY:13:PHE:HB3   | 61:B2:865:A:H5'   | 2.01                     | 0.43              |
| 26:AJ:108:GLU:O    | 26:AJ:114:GLN:NE2 | 2.48                     | 0.43              |
| 28:CN:167:ALA:O    | 28:CN:171:SER:N   | 2.51                     | 0.43              |
| 28:CN:184:ILE:HD12 | 28:CN:184:ILE:HA  | 1.84                     | 0.43              |
| 35:CP:174:LYS:HE3  | 62:A5:3848:U:C2   | 2.53                     | 0.43              |
| 46:Ci:60:HIS:ND1   | 46:Ci:64:GLU:OE2  | 2.45                     | 0.43              |
| 51:Cp:51:VAL:H     | 51:Cp:54:ILE:HG23 | 1.84                     | 0.43              |
| 51:Cp:77:ALA:O     | 51:Cp:81:SER:N    | 2.49                     | 0.43              |
| 59:A8:35:G:OP1     | 83:Cj:66:TYR:HE2  | 2.01                     | 0.43              |
| 61:B2:422:A:H5'    | 61:B2:423:G:C8    | 2.54                     | 0.43              |
| 61:B2:1142:U:O2    | 61:B2:1151:G:N2   | 2.39                     | 0.43              |
| 61:B2:1425:U:N3    | 61:B2:1579:G:O6   | 2.51                     | 0.43              |
| 61:B2:1540:G:H5'   | 69:AT:7:LYS:HZ1   | 1.83                     | 0.43              |
| 61:B2:1864:G:H2'   | 61:B2:1865:G:C8   | 2.53                     | 0.43              |
| 61:B2:1955:G:N2    | 61:B2:1977:A:N3   | 2.66                     | 0.43              |
| 62:A5:176:A:H1'    | 62:A5:272:U:H3    | 1.84                     | 0.43              |
| 62:A5:330:C:H2'    | 62:A5:331:A:C8    | 2.53                     | 0.43              |
| 62:A5:674:A:H2'    | 62:A5:675:C:H6    | 1.83                     | 0.43              |
| 62:A5:787:C:O2'    | 62:A5:788:C:OP2   | 2.33                     | 0.43              |
| 62:A5:1122:U:H5    | 62:A5:1123:C:H41  | 1.67                     | 0.43              |
| 62:A5:3265:C:H2'   | 62:A5:3266:A:C8   | 2.53                     | 0.43              |
| 69:AT:56:ARG:O     | 69:AT:59:SER:OG   | 2.30                     | 0.43              |
| 79:CV:45:ILE:HD12  | 79:CV:51:ARG:HH12 | 1.83                     | 0.43              |
| 80:CM:13:ALA:HA    | 80:CM:58:THR:HG23 | 2.00                     | 0.43              |
| 80:CM:96:GLN:O     | 80:CM:100:LYS:N   | 2.51                     | 0.43              |
| 2:CA:21:LYS:HD2    | 2:CA:21:LYS:HA    | 1.78                     | 0.43              |
| 3:AB:183:ASP:HA    | 3:AB:187:LEU:HB2  | 2.00                     | 0.43              |
| 5:AC:96:GLN:HE22   | 5:AC:105:THR:HG23 | 1.84                     | 0.43              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 6:CC:9:LEU:HD23    | 6:CC:9:LEU:HA     | 1.85                     | 0.43              |
| 15:AL:91:HIS:HB3   | 15:AL:100:GLU:HG2 | 2.01                     | 0.43              |
| 17:AP:82:HIS:HA    | 17:AP:100:TYR:HB3 | 2.00                     | 0.43              |
| 19:AY:79:THR:OG1   | 19:AY:80:LEU:N    | 2.51                     | 0.43              |
| 20:AZ:40:ARG:NH1   | 61:B2:1729:C:OP1  | 2.44                     | 0.43              |
| 21:Aa:45:VAL:HB    | 21:Aa:49:ALA:HB3  | 2.00                     | 0.43              |
| 26:AJ:116:PHE:HA   | 26:AJ:121:ALA:HB3 | 1.99                     | 0.43              |
| 33:CS:45:TRP:HE1   | 33:CS:61:ILE:HD11 | 1.83                     | 0.43              |
| 35:CP:174:LYS:NZ   | 62:A5:3849:A:O2'  | 2.48                     | 0.43              |
| 41:Cb:22:LYS:HA    | 41:Cb:22:LYS:HD2  | 1.80                     | 0.43              |
| 45:Cf:11:ALA:O     | 45:Cf:15:ALA:N    | 2.51                     | 0.43              |
| 46:Ci:13:LYS:HZ2   | 62:A5:77:A:P      | 2.41                     | 0.43              |
| 48:Cl:22:SER:OG    | 48:Cl:41:ARG:NH1  | 2.51                     | 0.43              |
| 54:CH:22:ALA:HB1   | 62:A5:3730:G:H5'  | 1.99                     | 0.43              |
| 55:CE:100:VAL:HG11 | 55:CE:221:PHE:HB2 | 2.01                     | 0.43              |
| 60:Cz:147:LYS:HA   | 60:Cz:147:LYS:HD3 | 1.67                     | 0.43              |
| 61:B2:2:U:O2'      | 61:B2:1186:U:O4   | 2.32                     | 0.43              |
| 61:B2:311:U:H2'    | 61:B2:312:G:C8    | 2.53                     | 0.43              |
| 61:B2:405:A:C6     | 75:AI:26:LYS:HG2  | 2.52                     | 0.43              |
| 61:B2:465:A:H3'    | 61:B2:466:G:H8    | 1.83                     | 0.43              |
| 61:B2:1260:G:H21   | 69:AT:88:HIS:CE1  | 2.37                     | 0.43              |
| 61:B2:1809:U:H1'   | 63:Ac:19:SER:HA   | 2.01                     | 0.43              |
| 62:A5:194:A:H2'    | 62:A5:195:A:C8    | 2.53                     | 0.43              |
| 62:A5:467:A:N6     | 62:A5:534:U:O4    | 2.51                     | 0.43              |
| 62:A5:793:U:OP1    | 62:A5:1153:G:N1   | 2.52                     | 0.43              |
| 62:A5:1017:A:C8    | 83:Cj:15:THR:HG21 | 2.11                     | 0.43              |
| 64:AW:17:ALA:O     | 64:AW:22:LYS:N    | 2.40                     | 0.43              |
| 69:AT:33:GLN:O     | 69:AT:37:VAL:HG23 | 2.19                     | 0.43              |
| 73:AG:88:ARG:N     | 73:AG:91:GLU:OE1  | 2.51                     | 0.43              |
| 74:AH:139:GLY:O    | 74:AH:155:HIS:ND1 | 2.45                     | 0.43              |
| 74:AH:141:ARG:HG3  | 74:AH:155:HIS:CE1 | 2.53                     | 0.43              |
| 74:AH:168:VAL:HA   | 74:AH:171:PHE:HB2 | 2.00                     | 0.43              |
| 76:AQ:83:ILE:O     | 76:AQ:87:ARG:NH1  | 2.51                     | 0.43              |
| 1:AA:42:ARG:HB2    | 1:AA:48:ILE:HD11  | 2.00                     | 0.43              |
| 2:CA:206:PRO:HG3   | 62:A5:3498:A:H4'  | 1.99                     | 0.43              |
| 4:CB:10:ARG:NH2    | 62:A5:3415:U:OP1  | 2.51                     | 0.43              |
| 4:CB:220:VAL:HA    | 4:CB:278:THR:HB   | 2.01                     | 0.43              |
| 4:CB:322:HIS:O     | 4:CB:342:LYS:NZ   | 2.45                     | 0.43              |
| 6:CC:65:THR:HG21   | 6:CC:95:PHE:CE1   | 2.54                     | 0.43              |
| 6:CC:275:THR:OG1   | 6:CC:276:LEU:N    | 2.52                     | 0.43              |
| 7:Ag:257:ILE:N     | 7:Ag:271:LEU:O    | 2.51                     | 0.43              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 9:AO:93:LEU:H      | 9:AO:126:ILE:HG22 | 1.84                     | 0.43              |
| 10:AX:11:ARG:NH2   | 61:B2:356:C:O4'   | 2.51                     | 0.43              |
| 17:AP:11:LYS:HG3   | 17:AP:13:ARG:HG2  | 1.99                     | 0.43              |
| 27:Ca:74:ILE:HD12  | 27:Ca:109:TYR:CG  | 2.54                     | 0.43              |
| 28:CN:136:ASP:OD2  | 57:A9:15:A:O2'    | 2.29                     | 0.43              |
| 34:CT:52:LEU:HD23  | 34:CT:95:HIS:CE1  | 2.53                     | 0.43              |
| 35:CP:29:THR:OG1   | 35:CP:87:SER:OG   | 2.24                     | 0.43              |
| 35:CP:96:ARG:O     | 35:CP:100:ALA:N   | 2.44                     | 0.43              |
| 40:Ch:109:ARG:O    | 40:Ch:112:SER:OG  | 2.35                     | 0.43              |
| 53:CJ:145:ASN:O    | 53:CJ:149:ARG:N   | 2.51                     | 0.43              |
| 54:CH:21:LYS:HD3   | 54:CH:21:LYS:HA   | 1.80                     | 0.43              |
| 56:CG:56:LEU:HD21  | 62:A5:2918:A:C4   | 2.52                     | 0.43              |
| 56:CG:212:VAL:O    | 56:CG:217:LYS:NZ  | 2.52                     | 0.43              |
| 59:A8:48:G:H2'     | 59:A8:49:C:C6     | 2.54                     | 0.43              |
| 61:B2:1467:U:H2'   | 61:B2:1468:G:C8   | 2.53                     | 0.43              |
| 62:A5:510:U:H2'    | 62:A5:511:G:H8    | 1.82                     | 0.43              |
| 62:A5:545:U:H2'    | 62:A5:546:G:C8    | 2.53                     | 0.43              |
| 62:A5:795:A:H1'    | 62:A5:797:A:N7    | 2.34                     | 0.43              |
| 62:A5:836:G:H2'    | 62:A5:837:A:C8    | 2.53                     | 0.43              |
| 62:A5:891:U:O4     | 62:A5:892:A:N6    | 2.51                     | 0.43              |
| 62:A5:928:U:O2'    | 62:A5:930:U:O5'   | 2.36                     | 0.43              |
| 62:A5:929:A:H8     | 62:A5:930:U:H4'   | 1.82                     | 0.43              |
| 62:A5:1017:A:C2    | 83:Cj:11:ARG:O    | 2.71                     | 0.43              |
| 62:A5:1120:A:OP1   | 62:A5:1123:C:N4   | 2.52                     | 0.43              |
| 62:A5:2004:G:H2'   | 62:A5:2005:U:C2   | 2.54                     | 0.43              |
| 62:A5:3344:U:H2'   | 62:A5:3345:A:H8   | 1.82                     | 0.43              |
| 65:CW:58:LYS:HB3   | 65:CW:58:LYS:HE3  | 1.83                     | 0.43              |
| 72:AE:82:TYR:HA    | 72:AE:83:PRO:HD3  | 1.88                     | 0.43              |
| 72:AE:194:THR:OG1  | 72:AE:211:LYS:NZ  | 2.42                     | 0.43              |
| 77:CO:8:THR:OG1    | 77:CO:9:VAL:N     | 2.51                     | 0.43              |
| 77:CO:198:ILE:HD12 | 77:CO:202:GLY:HA2 | 1.99                     | 0.43              |
| 80:CM:124:THR:HA   | 80:CM:127:PHE:HB2 | 2.01                     | 0.43              |
| 81:B:3:C:H2'       | 81:B:4:A:C8       | 2.52                     | 0.43              |
| 2:CA:19:HIS:NE2    | 2:CA:194:ASN:HB2  | 2.34                     | 0.43              |
| 2:CA:231:ALA:HA    | 2:CA:232:GLY:HA2  | 1.64                     | 0.43              |
| 3:AB:32:ASP:HA     | 3:AB:46:LYS:HD3   | 2.00                     | 0.43              |
| 3:AB:39:PHE:HB2    | 3:AB:74:LEU:HD12  | 2.01                     | 0.43              |
| 3:AB:128:VAL:HG13  | 3:AB:140:VAL:HB   | 1.99                     | 0.43              |
| 4:CB:45:CYS:SG     | 4:CB:183:ILE:HG12 | 2.59                     | 0.43              |
| 4:CB:118:PHE:O     | 62:A5:3535:G:O2'  | 2.37                     | 0.43              |
| 7:Ag:21:ILE:HA     | 7:Ag:33:SER:HA    | 2.01                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 7:Ag:113:ALA:HB3   | 7:Ag:122:VAL:HG13  | 2.00                     | 0.43              |
| 15:AL:28:LYS:HE2   | 15:AL:28:LYS:HB2   | 1.91                     | 0.43              |
| 15:AL:65:ILE:HD13  | 15:AL:128:CYS:HB3  | 2.00                     | 0.43              |
| 17:AP:78:ILE:HA    | 17:AP:107:GLN:HE22 | 1.83                     | 0.43              |
| 18:AV:40:ASP:HB2   | 18:AV:45:ARG:HB2   | 2.01                     | 0.43              |
| 19:AY:22:LYS:N     | 19:AY:76:ILE:O     | 2.51                     | 0.43              |
| 23:AD:110:LYS:HD3  | 23:AD:110:LYS:HA   | 1.82                     | 0.43              |
| 26:AJ:130:LEU:HD12 | 26:AJ:135:HIS:HB2  | 2.01                     | 0.43              |
| 27:Ca:41:HIS:HB2   | 62:A5:1158:C:H1'   | 2.00                     | 0.43              |
| 28:CN:73:ARG:H     | 28:CN:89:VAL:HG13  | 1.83                     | 0.43              |
| 31:CQ:91:ARG:H     | 31:CQ:91:ARG:HG3   | 1.57                     | 0.43              |
| 43:Cd:62:ASP:OD2   | 43:Cd:102:TYR:OH   | 2.28                     | 0.43              |
| 48:Cl:18:LYS:NZ    | 59:A8:46:C:OP2     | 2.51                     | 0.43              |
| 60:Cz:213:PRO:HG2  | 62:A5:2886:C:H5'   | 2.00                     | 0.43              |
| 61:B2:63:G:O2'     | 61:B2:167:U:OP1    | 2.37                     | 0.43              |
| 61:B2:856:A:OP2    | 61:B2:871:G:N1     | 2.36                     | 0.43              |
| 62:A5:454:C:O2     | 62:A5:773:G:N2     | 2.52                     | 0.43              |
| 62:A5:1186:U:H5''  | 71:CF:180:ARG:HA   | 2.00                     | 0.43              |
| 66:Cg:2:VAL:HG11   | 66:Cg:30:LEU:HD11  | 2.01                     | 0.43              |
| 69:AT:126:ILE:HG22 | 69:AT:131:LEU:CD1  | 2.46                     | 0.43              |
| 73:AG:3:LEU:N      | 73:AG:16:PHE:O     | 2.51                     | 0.43              |
| 77:CO:33:GLY:H     | 77:CO:103:ARG:NH1  | 2.17                     | 0.43              |
| 2:CA:185:ALA:HA    | 2:CA:188:LYS:HB3   | 2.00                     | 0.43              |
| 4:CB:285:TYR:HD1   | 4:CB:285:TYR:HA    | 1.70                     | 0.43              |
| 6:CC:238:LEU:HD23  | 6:CC:238:LEU:HA    | 1.85                     | 0.43              |
| 8:AU:53:LYS:NZ     | 61:B2:1546:U:O2    | 2.45                     | 0.43              |
| 8:AU:84:MET:HE3    | 8:AU:84:MET:HB3    | 1.84                     | 0.43              |
| 11:AM:59:LEU:HD22  | 11:AM:69:LYS:HB2   | 2.01                     | 0.43              |
| 15:AL:93:VAL:HG21  | 15:AL:96:TYR:HD2   | 1.84                     | 0.43              |
| 17:AP:33:ASN:ND2   | 17:AP:34:ASN:OD1   | 2.52                     | 0.43              |
| 23:AD:8:SER:O      | 23:AD:12:LYS:N     | 2.50                     | 0.43              |
| 27:Ca:69:LYS:NZ    | 62:A5:861:C:OP1    | 2.51                     | 0.43              |
| 29:CI:38:ARG:HD2   | 29:CI:41:ALA:HB2   | 2.01                     | 0.43              |
| 30:CD:17:GLN:HE22  | 34:CT:22:HIS:H     | 1.65                     | 0.43              |
| 30:CD:119:TYR:OH   | 30:CD:139:PRO:O    | 2.37                     | 0.43              |
| 32:CR:160:GLU:HB3  | 32:CR:163:ARG:HE   | 1.84                     | 0.43              |
| 36:CX:168:ARG:HH11 | 62:A5:1804:A:H61   | 1.66                     | 0.43              |
| 40:Ch:96:SER:O     | 40:Ch:100:ALA:N    | 2.52                     | 0.43              |
| 40:Ch:118:LYS:HA   | 78:CL:48:ARG:HH12  | 1.84                     | 0.43              |
| 46:CI:16:LYS:HE3   | 46:CI:16:LYS:HB3   | 1.85                     | 0.43              |
| 48:Cl:20:ASN:OD1   | 48:Cl:20:ASN:N     | 2.51                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 55:CE:16:LYS:NZ   | 62:A5:693:G:OP1   | 2.39                     | 0.43              |
| 55:CE:195:ASN:HB3 | 55:CE:198:ARG:HG3 | 2.01                     | 0.43              |
| 57:A9:15:A:H61    | 62:A5:21:U:H3     | 1.66                     | 0.43              |
| 61:B2:377:G:C6    | 61:B2:378:G:H1'   | 2.54                     | 0.43              |
| 61:B2:949:A:H4'   | 64:AW:57:ARG:HB3  | 1.99                     | 0.43              |
| 61:B2:1636:A:H4'  | 61:B2:1637:G:H3'  | 2.01                     | 0.43              |
| 62:A5:551:C:H42   | 62:A5:661:G:H1    | 1.67                     | 0.43              |
| 62:A5:1016:A:H5'  | 62:A5:1120:A:H62  | 1.83                     | 0.43              |
| 62:A5:1558:A:H2'  | 62:A5:1559:A:H8   | 1.84                     | 0.43              |
| 62:A5:1890:U:O2   | 66:Cg:8:ARG:NH1   | 2.51                     | 0.43              |
| 62:A5:1904:G:H2'  | 62:A5:1905:A:H8   | 1.83                     | 0.43              |
| 62:A5:2251:G:H2'  | 62:A5:2252:A:H8   | 1.84                     | 0.43              |
| 62:A5:3377:A:H2   | 62:A5:3382:G:H1   | 1.66                     | 0.43              |
| 62:A5:3896:G:N2   | 62:A5:3960:U:O2   | 2.51                     | 0.43              |
| 72:AE:180:LEU:O   | 72:AE:228:ILE:N   | 2.42                     | 0.43              |
| 78:CL:107:GLU:HA  | 78:CL:110:GLN:HB2 | 2.01                     | 0.43              |
| 80:CM:137:ASP:HB2 | 80:CM:141:ARG:HD2 | 2.01                     | 0.43              |
| 2:CA:176:ASP:HB3  | 51:Cp:29:MET:HE1  | 2.00                     | 0.43              |
| 2:CA:207:VAL:HG12 | 62:A5:2793:C:H4'  | 2.01                     | 0.43              |
| 2:CA:226:LYS:HE2  | 2:CA:226:LYS:HB3  | 1.84                     | 0.43              |
| 16:AR:79:GLU:O    | 16:AR:80:ARG:NH1  | 2.51                     | 0.43              |
| 20:AZ:51:LYS:HE2  | 20:AZ:51:LYS:HB2  | 1.83                     | 0.43              |
| 30:CD:94:ASN:HB2  | 30:CD:97:ALA:H    | 1.84                     | 0.43              |
| 30:CD:217:GLU:HA  | 30:CD:220:LYS:HB2 | 2.01                     | 0.43              |
| 38:CZ:116:LYS:O   | 38:CZ:119:SER:OG  | 2.26                     | 0.43              |
| 50:Cn:1:MET:N     | 61:B2:1978:C:OP1  | 2.33                     | 0.43              |
| 55:CE:35:LYS:HA   | 55:CE:35:LYS:HD2  | 1.85                     | 0.43              |
| 55:CE:164:ASN:H   | 55:CE:167:TYR:HB3 | 1.83                     | 0.43              |
| 61:B2:139:U:H2'   | 61:B2:140:G:C8    | 2.54                     | 0.43              |
| 61:B2:719:G:H22   | 61:B2:818:C:H2'   | 1.84                     | 0.43              |
| 61:B2:1025:G:N3   | 61:B2:1029:G:N2   | 2.67                     | 0.43              |
| 62:A5:82:U:H2'    | 62:A5:83:U:H6     | 1.84                     | 0.43              |
| 62:A5:313:A:H61   | 62:A5:335:A:H61   | 1.67                     | 0.43              |
| 62:A5:487:A:N6    | 62:A5:513:G:H1    | 2.14                     | 0.43              |
| 62:A5:591:A:N6    | 62:A5:620:U:O4    | 2.52                     | 0.43              |
| 62:A5:1954:G:H3'  | 66:Cg:68:ARG:HE   | 1.83                     | 0.43              |
| 62:A5:2175:A:O2'  | 66:Cg:1:MET:SD    | 2.64                     | 0.43              |
| 74:AH:32:ASN:HD21 | 74:AH:35:LEU:HD23 | 1.84                     | 0.43              |
| 4:CB:161:ARG:HG2  | 4:CB:184:GLN:HB2  | 2.01                     | 0.43              |
| 6:CC:175:ARG:HH22 | 62:A5:224:U:H2'   | 1.84                     | 0.43              |
| 11:AM:56:LEU:HA   | 11:AM:82:PRO:HB2  | 2.01                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 12:AS:38:ARG:HB3   | 69:AT:45:LEU:CD2   | 2.49                     | 0.43              |
| 14:AN:35:GLU:O     | 14:AN:39:LYS:N     | 2.51                     | 0.43              |
| 15:AL:27:LYS:O     | 15:AL:27:LYS:NZ    | 2.52                     | 0.43              |
| 26:AJ:114:GLN:OE1  | 26:AJ:155:GLN:NE2  | 2.52                     | 0.43              |
| 26:AJ:137:ARG:HH21 | 26:AJ:162:LEU:H    | 1.67                     | 0.43              |
| 28:CN:56:LYS:HB3   | 28:CN:56:LYS:HE2   | 1.75                     | 0.43              |
| 28:CN:143:ARG:NH1  | 62:A5:141:U:O2     | 2.46                     | 0.43              |
| 33:CS:78:PHE:HD1   | 33:CS:131:SER:HA   | 1.84                     | 0.43              |
| 33:CS:101:THR:OG1  | 33:CS:102:VAL:N    | 2.52                     | 0.43              |
| 34:CT:7:TYR:HB3    | 34:CT:54:TYR:HE2   | 1.82                     | 0.43              |
| 34:CT:41:ASP:OD1   | 34:CT:42:ILE:N     | 2.52                     | 0.43              |
| 48:Cl:18:LYS:HB2   | 48:Cl:18:LYS:HE3   | 1.81                     | 0.43              |
| 55:CE:112:ARG:NH1  | 55:CE:228:ASN:O    | 2.52                     | 0.43              |
| 56:CG:160:VAL:HA   | 56:CG:208:ALA:HA   | 1.99                     | 0.43              |
| 58:A7:3:C:H2'      | 58:A7:4:A:C8       | 2.54                     | 0.43              |
| 61:B2:296:G:H2'    | 61:B2:297:A:C8     | 2.54                     | 0.43              |
| 61:B2:469:A:H2'    | 61:B2:470:G:H8     | 1.84                     | 0.43              |
| 61:B2:1381:G:N2    | 61:B2:1409:A:O5'   | 2.51                     | 0.43              |
| 61:B2:1717:A:O4'   | 69:AT:92:PHE:CZ    | 2.71                     | 0.43              |
| 62:A5:164:U:H1'    | 78:CL:100:ARG:HB2  | 2.00                     | 0.43              |
| 62:A5:775:U:H2'    | 62:A5:776:A:C8     | 2.54                     | 0.43              |
| 62:A5:794:G:H2'    | 62:A5:2750:A:C5    | 2.54                     | 0.43              |
| 62:A5:1137:G:C8    | 62:A5:1137:G:H5'   | 2.53                     | 0.43              |
| 62:A5:1176:A:H2'   | 62:A5:1177:U:C6    | 2.54                     | 0.43              |
| 69:AT:127:GLY:O    | 69:AT:132:ASP:OD2  | 2.36                     | 0.43              |
| 69:AT:137:GLN:O    | 69:AT:141:LYS:HG3  | 2.19                     | 0.43              |
| 73:AG:78:LYS:O     | 73:AG:81:HIS:ND1   | 2.38                     | 0.43              |
| 76:AQ:23:ALA:HA    | 76:AQ:74:VAL:HG22  | 2.01                     | 0.43              |
| 4:CB:220:VAL:HG13  | 4:CB:278:THR:HB    | 2.00                     | 0.42              |
| 5:AC:192:VAL:HG21  | 5:AC:216:LEU:HD11  | 2.01                     | 0.42              |
| 7:Ag:71:VAL:HG22   | 7:Ag:112:VAL:HG13  | 2.01                     | 0.42              |
| 11:AM:63:PHE:HB3   | 11:AM:69:LYS:HD2   | 2.00                     | 0.42              |
| 11:AM:133:ASP:OD1  | 11:AM:133:ASP:N    | 2.52                     | 0.42              |
| 28:CN:27:VAL:HG13  | 28:CN:28:TRP:HD1   | 1.84                     | 0.42              |
| 28:CN:31:ARG:HH21  | 28:CN:127:TYR:HB2  | 1.83                     | 0.42              |
| 29:Cl:15:LYS:HE2   | 62:A5:1339:U:H5'   | 2.00                     | 0.42              |
| 34:CT:87:LYS:HD2   | 34:CT:87:LYS:HA    | 1.71                     | 0.42              |
| 40:Ch:122:LYS:HB3  | 78:CL:149:LEU:HD12 | 2.01                     | 0.42              |
| 45:Cf:82:GLU:HB3   | 55:CE:240:ARG:HH22 | 1.83                     | 0.42              |
| 48:Cl:33:ASN:OD1   | 48:Cl:33:ASN:N     | 2.52                     | 0.42              |
| 53:CJ:4:VAL:O      | 58:A7:19:C:O2'     | 2.29                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 55:CE:172:LYS:HD3 | 55:CE:172:LYS:HA  | 1.77                     | 0.42              |
| 59:A8:44:C:H2'    | 59:A8:45:G:H8     | 1.83                     | 0.42              |
| 61:B2:527:C:H3'   | 61:B2:528:A:H8    | 1.83                     | 0.42              |
| 62:A5:268:U:H2'   | 62:A5:269:A:C8    | 2.53                     | 0.42              |
| 62:A5:1009:G:H22  | 62:A5:1131:C:N4   | 2.17                     | 0.42              |
| 62:A5:1617:U:H2'  | 62:A5:1618:A:C8   | 2.54                     | 0.42              |
| 62:A5:2904:U:H2'  | 62:A5:2905:A:H8   | 1.84                     | 0.42              |
| 62:A5:3519:C:H2'  | 62:A5:3520:U:C6   | 2.54                     | 0.42              |
| 63:Ac:29:GLU:HB3  | 63:Ac:37:GLN:HG3  | 2.01                     | 0.42              |
| 67:CU:213:GLN:HA  | 67:CU:216:LYS:HB3 | 2.00                     | 0.42              |
| 71:CF:144:THR:HA  | 71:CF:238:GLY:H   | 1.83                     | 0.42              |
| 3:AB:27:ARG:HE    | 3:AB:51:ARG:HD3   | 1.84                     | 0.42              |
| 6:CC:66:SER:OG    | 62:A5:1129:A:OP2  | 2.36                     | 0.42              |
| 7:Ag:31:ILE:HD12  | 7:Ag:45:LEU:HD21  | 2.00                     | 0.42              |
| 12:AS:85:ASN:HB2  | 12:AS:97:GLN:HA   | 2.00                     | 0.42              |
| 12:AS:137:LYS:HE3 | 12:AS:137:LYS:HB3 | 1.93                     | 0.42              |
| 13:Ad:48:ASN:HA   | 13:Ad:50:ILE:H    | 1.84                     | 0.42              |
| 22:Ab:23:ARG:HH12 | 22:Ab:27:HIS:HB3  | 1.84                     | 0.42              |
| 27:Ca:87:LYS:HD3  | 78:CL:166:PHE:CG  | 2.54                     | 0.42              |
| 27:Ca:98:LYS:HA   | 27:Ca:98:LYS:HD3  | 1.67                     | 0.42              |
| 34:CT:41:ASP:OD2  | 62:A5:1204:C:O2'  | 2.37                     | 0.42              |
| 36:CX:162:ARG:HG2 | 62:A5:1813:A:N7   | 2.34                     | 0.42              |
| 38:CZ:121:TYR:O   | 38:CZ:127:LYS:NZ  | 2.53                     | 0.42              |
| 43:Cd:38:ARG:HG2  | 43:Cd:39:ALA:HB2  | 2.01                     | 0.42              |
| 51:Cp:78:SER:O    | 51:Cp:82:ALA:N    | 2.52                     | 0.42              |
| 53:CJ:100:ARG:NH2 | 53:CJ:182:THR:O   | 2.51                     | 0.42              |
| 56:CG:214:ASN:HA  | 56:CG:217:LYS:HE2 | 2.01                     | 0.42              |
| 61:B2:562:C:N4    | 61:B2:579:G:O6    | 2.51                     | 0.42              |
| 61:B2:953:A:H2'   | 61:B2:954:A:H8    | 1.84                     | 0.42              |
| 61:B2:1063:G:N1   | 61:B2:1110:A:O2'  | 2.47                     | 0.42              |
| 61:B2:1236:C:O2   | 61:B2:1241:G:N2   | 2.40                     | 0.42              |
| 61:B2:1362:A:N7   | 61:B2:1623:C:N4   | 2.51                     | 0.42              |
| 61:B2:1453:G:N1   | 61:B2:1533:C:O2   | 2.51                     | 0.42              |
| 62:A5:1459:A:N6   | 62:A5:1463:C:OP2  | 2.52                     | 0.42              |
| 62:A5:1910:C:H2'  | 62:A5:1924:A:H4'  | 2.01                     | 0.42              |
| 62:A5:3448:U:N3   | 62:A5:3467:A:N7   | 2.67                     | 0.42              |
| 62:A5:3602:U:O4   | 62:A5:3603:C:N4   | 2.51                     | 0.42              |
| 66:Cg:51:LEU:HD23 | 66:Cg:51:LEU:HA   | 1.76                     | 0.42              |
| 67:CU:216:LYS:NZ  | 67:CU:226:ASN:OD1 | 2.53                     | 0.42              |
| 68:AK:43:VAL:O    | 68:AK:48:GLN:NE2  | 2.44                     | 0.42              |
| 69:AT:30:VAL:HG12 | 69:AT:31:PRO:O    | 2.18                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 69:AT:85:ASN:ND2   | 69:AT:91:HIS:O     | 2.53                     | 0.42              |
| 69:AT:133:ARG:HA   | 69:AT:136:ASN:HB2  | 2.01                     | 0.42              |
| 70:AF:221:GLU:HA   | 70:AF:224:ALA:HB3  | 2.01                     | 0.42              |
| 74:AH:107:ARG:HD2  | 74:AH:107:ARG:HA   | 1.72                     | 0.42              |
| 80:CM:9:THR:HA     | 80:CM:27:ILE:HG23  | 2.01                     | 0.42              |
| 80:CM:127:PHE:HD1  | 80:CM:127:PHE:HA   | 1.72                     | 0.42              |
| 6:CC:368:SER:O     | 6:CC:372:ASN:ND2   | 2.53                     | 0.42              |
| 7:Ag:266:LYS:HZ1   | 7:Ag:268:VAL:HG22  | 1.83                     | 0.42              |
| 9:AO:140:THR:HG21  | 61:B2:974:A:C2     | 2.54                     | 0.42              |
| 15:AL:122:ILE:HD13 | 15:AL:144:LYS:HD3  | 2.01                     | 0.42              |
| 18:AV:69:ILE:HD12  | 18:AV:72:LEU:HD12  | 2.00                     | 0.42              |
| 27:Ca:79:LEU:H     | 27:Ca:82:LEU:HD13  | 1.83                     | 0.42              |
| 28:CN:73:ARG:NH1   | 62:A5:37:G:OP1     | 2.52                     | 0.42              |
| 28:CN:147:LYS:HE3  | 28:CN:147:LYS:HB2  | 1.83                     | 0.42              |
| 31:CQ:28:LEU:HD23  | 31:CQ:28:LEU:HA    | 1.79                     | 0.42              |
| 31:CQ:152:PHE:CD1  | 62:A5:1322:U:H4'   | 2.55                     | 0.42              |
| 33:CS:96:GLU:HG2   | 33:CS:139:ARG:HG3  | 2.01                     | 0.42              |
| 34:CT:138:ALA:HB2  | 71:CF:88:ALA:HB2   | 2.01                     | 0.42              |
| 36:CX:178:SER:OG   | 36:CX:180:LYS:NZ   | 2.52                     | 0.42              |
| 37:CY:35:SER:HA    | 37:CY:105:LEU:HD11 | 2.00                     | 0.42              |
| 39:Cr:60:ASP:OD1   | 39:Cr:60:ASP:N     | 2.37                     | 0.42              |
| 54:CH:91:ARG:HH11  | 54:CH:141:GLU:HG3  | 1.84                     | 0.42              |
| 56:CG:266:LEU:HA   | 56:CG:269:LYS:HG2  | 2.00                     | 0.42              |
| 59:A8:26:U:H3      | 62:A5:355:G:H22    | 1.67                     | 0.42              |
| 61:B2:1136:U:H2'   | 61:B2:1137:G:C8    | 2.54                     | 0.42              |
| 61:B2:1715:G:O3'   | 69:AT:78:ILE:HG21  | 2.19                     | 0.42              |
| 62:A5:1017:A:H2    | 83:Cj:11:ARG:O     | 2.02                     | 0.42              |
| 62:A5:1691:A:C2    | 62:A5:1692:G:H1'   | 2.54                     | 0.42              |
| 62:A5:1735:G:O2'   | 62:A5:2159:C:H5''  | 2.19                     | 0.42              |
| 62:A5:2174:A:H5'   | 66:Cg:4:ARG:HG2    | 2.01                     | 0.42              |
| 62:A5:3728:A:H8    | 62:A5:3729:A:H4'   | 1.84                     | 0.42              |
| 62:A5:3896:G:H2'   | 62:A5:3897:G:C8    | 2.54                     | 0.42              |
| 70:AF:200:GLU:O    | 70:AF:204:ALA:N    | 2.47                     | 0.42              |
| 73:AG:131:ARG:HA   | 73:AG:131:ARG:HD3  | 1.81                     | 0.42              |
| 6:CC:32:LYS:HZ3    | 6:CC:270:TRP:CD1   | 2.37                     | 0.42              |
| 6:CC:77:ALA:HA     | 62:A5:1677:U:C5    | 2.54                     | 0.42              |
| 17:AP:57:MET:HA    | 17:AP:60:ILE:HD12  | 2.00                     | 0.42              |
| 22:Ab:55:VAL:HA    | 22:Ab:63:LEU:HD13  | 2.00                     | 0.42              |
| 33:CS:160:HIS:NE2  | 62:A5:1396:A:O4'   | 2.49                     | 0.42              |
| 35:CP:178:GLN:HE22 | 45:Cf:111:LYS:HZ1  | 1.66                     | 0.42              |
| 38:CZ:11:VAL:HB    | 38:CZ:80:LEU:HD12  | 2.01                     | 0.42              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 38:CZ:24:ILE:N     | 38:CZ:44:ALA:O    | 2.41                     | 0.42              |
| 38:CZ:64:LYS:HB2   | 62:A5:2126:A:H61  | 1.84                     | 0.42              |
| 38:CZ:91:SER:O     | 38:CZ:94:LYS:NZ   | 2.50                     | 0.42              |
| 38:CZ:92:PHE:CD2   | 38:CZ:116:LYS:HB2 | 2.54                     | 0.42              |
| 43:CD:38:ARG:HA    | 43:CD:39:ALA:HA   | 1.64                     | 0.42              |
| 44:CE:48:PHE:CE1   | 62:A5:1359:G:H5'  | 2.54                     | 0.42              |
| 45:CF:46:ARG:HH11  | 45:CF:49:ARG:NH2  | 2.17                     | 0.42              |
| 51:Cp:16:THR:O     | 51:Cp:16:THR:OG1  | 2.26                     | 0.42              |
| 55:CE:134:SER:OG   | 62:A5:3836:A:N3   | 2.49                     | 0.42              |
| 55:CE:193:VAL:HG13 | 55:CE:194:PRO:C   | 2.44                     | 0.42              |
| 56:CG:125:ALA:O    | 56:CG:129:GLY:N   | 2.52                     | 0.42              |
| 60:Cz:42:ASP:HA    | 60:Cz:43:PRO:HD3  | 1.90                     | 0.42              |
| 61:B2:255:U:OP2    | 61:B2:256:C:N4    | 2.49                     | 0.42              |
| 61:B2:274:G:N1     | 61:B2:291:C:O2    | 2.35                     | 0.42              |
| 61:B2:942:A:H2'    | 74:AH:118:ARG:NH2 | 2.34                     | 0.42              |
| 61:B2:1066:A:O2'   | 61:B2:1970:U:O2   | 2.37                     | 0.42              |
| 61:B2:1468:G:O6    | 61:B2:1520:A:N6   | 2.52                     | 0.42              |
| 61:B2:1727:U:C5    | 70:AF:190:ILE:CB  | 3.02                     | 0.42              |
| 62:A5:360:A:H8     | 62:A5:360:A:H5'   | 1.84                     | 0.42              |
| 62:A5:489:U:H3     | 62:A5:511:G:H22   | 1.68                     | 0.42              |
| 62:A5:796:A:N6     | 62:A5:2749:G:H21  | 2.14                     | 0.42              |
| 62:A5:839:A:O2'    | 62:A5:840:U:O5'   | 2.36                     | 0.42              |
| 62:A5:1643:G:H2'   | 62:A5:1644:C:C6   | 2.55                     | 0.42              |
| 62:A5:1908:A:OP1   | 62:A5:2134:A:N6   | 2.52                     | 0.42              |
| 62:A5:2193:C:H5''  | 62:A5:2194:G:H5'  | 2.01                     | 0.42              |
| 69:AT:83:LYS:HZ3   | 69:AT:95:ALA:CA   | 2.32                     | 0.42              |
| 70:AF:63:ILE:HD13  | 70:AF:63:ILE:HA   | 1.89                     | 0.42              |
| 71:CF:188:ILE:HG23 | 71:CF:193:ASP:HB2 | 2.01                     | 0.42              |
| 71:CF:231:TYR:CD2  | 71:CF:240:ARG:HB3 | 2.54                     | 0.42              |
| 72:AE:239:PRO:O    | 72:AE:242:LYS:NZ  | 2.53                     | 0.42              |
| 75:AI:25:ARG:HD3   | 75:AI:25:ARG:HA   | 1.77                     | 0.42              |
| 78:CL:107:GLU:O    | 78:CL:111:ARG:N   | 2.53                     | 0.42              |
| 80:CM:5:ARG:CZ     | 80:CM:57:LEU:H    | 2.32                     | 0.42              |
| 80:CM:135:LYS:HE2  | 80:CM:135:LYS:HB2 | 1.88                     | 0.42              |
| 4:CB:39:LYS:HA     | 4:CB:39:LYS:HD2   | 1.72                     | 0.42              |
| 6:CC:234:ASN:OD1   | 6:CC:235:VAL:N    | 2.53                     | 0.42              |
| 8:AU:74:GLU:OE1    | 61:B2:1621:G:O2'  | 2.38                     | 0.42              |
| 10:AX:52:LEU:HD12  | 10:AX:71:ARG:HG2  | 2.01                     | 0.42              |
| 17:AP:101:ASN:OD1  | 17:AP:101:ASN:N   | 2.52                     | 0.42              |
| 23:AD:59:GLN:O     | 23:AD:67:ARG:NH1  | 2.52                     | 0.42              |
| 23:AD:118:ARG:HH12 | 24:Ae:124:ARG:HB2 | 1.84                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:Ca:45:ASN:HD22  | 27:Ca:45:ASN:C     | 2.27                     | 0.42              |
| 30:CD:205:ALA:HB2  | 30:CD:236:LEU:HD22 | 2.02                     | 0.42              |
| 31:CQ:64:GLN:HE22  | 31:CQ:91:ARG:HB2   | 1.85                     | 0.42              |
| 35:CP:92:LEU:HD23  | 35:CP:92:LEU:HA    | 1.82                     | 0.42              |
| 38:CZ:67:LYS:HD3   | 38:CZ:67:LYS:HA    | 1.86                     | 0.42              |
| 43:Cd:57:THR:OG1   | 43:Cd:58:ASP:N     | 2.51                     | 0.42              |
| 45:Cf:72:ILE:HD11  | 45:Cf:125:HIS:CD2  | 2.54                     | 0.42              |
| 47:Ck:55:LYS:HG3   | 47:Ck:56:ILE:HG12  | 2.01                     | 0.42              |
| 50:Cn:16:LYS:NZ    | 50:Cn:19:LYS:HD2   | 2.34                     | 0.42              |
| 52:Co:6:LYS:HD2    | 52:Co:7:GLN:HE21   | 1.84                     | 0.42              |
| 52:Co:31:GLU:HG3   | 62:A5:3298:U:H4'   | 2.01                     | 0.42              |
| 54:CH:62:LYS:HD3   | 54:CH:62:LYS:HA    | 1.87                     | 0.42              |
| 61:B2:355:G:H4'    | 61:B2:356:C:H5''   | 2.02                     | 0.42              |
| 61:B2:371:A:H61    | 61:B2:380:U:H3     | 1.68                     | 0.42              |
| 61:B2:477:A:O2'    | 61:B2:851:A:N3     | 2.51                     | 0.42              |
| 61:B2:718:C:O2'    | 61:B2:775:U:OP1    | 2.37                     | 0.42              |
| 61:B2:1716:A:P     | 69:AT:78:ILE:HG21  | 2.54                     | 0.42              |
| 62:A5:73:U:H3'     | 62:A5:74:A:C8      | 2.52                     | 0.42              |
| 62:A5:579:A:O2'    | 62:A5:633:A:N6     | 2.53                     | 0.42              |
| 62:A5:1101:A:H2'   | 62:A5:1102:G:C8    | 2.55                     | 0.42              |
| 62:A5:1292:G:N2    | 62:A5:1296:U:O2    | 2.40                     | 0.42              |
| 62:A5:2006:U:OP2   | 62:A5:2085:G:O2'   | 2.38                     | 0.42              |
| 62:A5:2262:A:H2'   | 62:A5:2263:A:H8    | 1.84                     | 0.42              |
| 62:A5:2807:G:H2'   | 62:A5:2808:G:H8    | 1.85                     | 0.42              |
| 62:A5:2921:G:H2'   | 62:A5:2922:G:H8    | 1.83                     | 0.42              |
| 62:A5:3005:A:H62   | 62:A5:3112:A:H62   | 1.67                     | 0.42              |
| 67:CU:221:ILE:HB   | 67:CU:228:LEU:HD13 | 2.00                     | 0.42              |
| 72:AE:10:LYS:HA    | 72:AE:27:PHE:HA    | 2.02                     | 0.42              |
| 73:AG:91:GLU:H     | 73:AG:91:GLU:HG2   | 1.72                     | 0.42              |
| 1:AA:214:GLU:HB3   | 1:AA:218:LYS:HE2   | 2.02                     | 0.42              |
| 3:AB:225:ARG:HH11  | 3:AB:227:ASP:H     | 1.67                     | 0.42              |
| 5:AC:125:LYS:HE2   | 5:AC:137:ALA:HB2   | 2.01                     | 0.42              |
| 5:AC:221:LYS:NZ    | 61:B2:1385:U:O3'   | 2.51                     | 0.42              |
| 6:CC:112:ARG:HB2   | 6:CC:114:TRP:CE3   | 2.55                     | 0.42              |
| 6:CC:263:LEU:HA    | 6:CC:266:LEU:HB2   | 2.01                     | 0.42              |
| 11:AM:52:ARG:NH1   | 11:AM:78:GLU:OE1   | 2.52                     | 0.42              |
| 12:AS:66:LYS:O     | 12:AS:69:THR:OG1   | 2.30                     | 0.42              |
| 13:Ad:56:ASP:OD1   | 61:B2:1610:A:O2'   | 2.38                     | 0.42              |
| 23:AD:125:LEU:HD13 | 23:AD:128:ILE:HD11 | 2.01                     | 0.42              |
| 24:Ae:85:LYS:HD3   | 61:B2:592:C:H4'    | 2.02                     | 0.42              |
| 27:Ca:117:HIS:ND1  | 62:A5:869:A:OP2    | 2.40                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 29:CI:101:LYS:HA  | 29:CI:101:LYS:HD2  | 1.83                     | 0.42              |
| 40:Ch:9:LEU:HD13  | 40:Ch:12:LYS:HD3   | 2.01                     | 0.42              |
| 46:CI:87:LEU:O    | 62:A5:290:G:N2     | 2.46                     | 0.42              |
| 48:CI:13:LEU:HD23 | 48:CI:13:LEU:HA    | 1.76                     | 0.42              |
| 54:CH:45:MET:SD   | 54:CH:45:MET:N     | 2.92                     | 0.42              |
| 54:CH:69:ARG:O    | 54:CH:73:SER:N     | 2.48                     | 0.42              |
| 58:A7:45:A:H2'    | 58:A7:46:C:C6      | 2.54                     | 0.42              |
| 61:B2:913:G:H2'   | 61:B2:914:C:H6     | 1.83                     | 0.42              |
| 61:B2:1094:C:H2'  | 61:B2:1095:G:C8    | 2.54                     | 0.42              |
| 61:B2:1590:G:H1   | 61:B2:1593:U:H5''  | 1.85                     | 0.42              |
| 62:A5:819:U:H2'   | 62:A5:820:A:C8     | 2.55                     | 0.42              |
| 62:A5:1634:A:H61  | 62:A5:1658:G:H1'   | 1.85                     | 0.42              |
| 62:A5:1872:A:N6   | 62:A5:2149:G:H1'   | 2.35                     | 0.42              |
| 62:A5:2019:U:H3   | 62:A5:2052:G:H1    | 1.66                     | 0.42              |
| 62:A5:3331:A:O2'  | 62:A5:3332:G:N7    | 2.46                     | 0.42              |
| 62:A5:3592:C:O2'  | 62:A5:3594:A:OP1   | 2.31                     | 0.42              |
| 73:AG:70:HIS:ND1  | 73:AG:103:ASP:OD2  | 2.49                     | 0.42              |
| 73:AG:132:ARG:HG3 | 73:AG:133:LEU:HD12 | 2.02                     | 0.42              |
| 73:AG:155:ARG:HD3 | 73:AG:155:ARG:HA   | 1.77                     | 0.42              |
| 2:CA:73:LYS:HE2   | 2:CA:73:LYS:HB2    | 1.92                     | 0.42              |
| 3:AB:225:ARG:NH1  | 3:AB:227:ASP:H     | 2.18                     | 0.42              |
| 5:AC:129:GLU:O    | 5:AC:132:THR:OG1   | 2.37                     | 0.42              |
| 11:AM:49:LEU:HB2  | 11:AM:75:LEU:HD22  | 2.02                     | 0.42              |
| 12:AS:88:LYS:HG3  | 12:AS:95:TYR:HE1   | 1.85                     | 0.42              |
| 15:AL:45:ARG:NH1  | 61:B2:932:U:O2'    | 2.51                     | 0.42              |
| 25:Af:95:ARG:NH2  | 61:B2:1320:G:N7    | 2.66                     | 0.42              |
| 25:Af:118:ARG:HA  | 25:Af:118:ARG:HD3  | 1.88                     | 0.42              |
| 27:Ca:12:LEU:HD23 | 27:Ca:12:LEU:HA    | 1.82                     | 0.42              |
| 30:CD:280:THR:O   | 30:CD:284:ALA:N    | 2.48                     | 0.42              |
| 33:CS:115:ALA:HB1 | 62:A5:1400:A:N3    | 2.35                     | 0.42              |
| 35:CP:34:GLN:NE2  | 35:CP:117:ILE:O    | 2.36                     | 0.42              |
| 39:Cr:32:GLU:OE2  | 39:Cr:45:SER:OG    | 2.34                     | 0.42              |
| 40:Ch:7:SER:HA    | 40:Ch:10:ARG:HE    | 1.84                     | 0.42              |
| 45:Cf:49:ARG:NH2  | 55:CE:232:LEU:O    | 2.53                     | 0.42              |
| 45:Cf:53:LYS:NZ   | 45:Cf:147:ARG:O    | 2.53                     | 0.42              |
| 45:Cf:113:ARG:HD2 | 45:Cf:113:ARG:HA   | 1.87                     | 0.42              |
| 54:CH:172:LYS:NZ  | 62:A5:3561:G:OP1   | 2.44                     | 0.42              |
| 55:CE:117:LYS:HZ3 | 55:CE:159:VAL:HB   | 1.84                     | 0.42              |
| 56:CG:39:LYS:NZ   | 62:A5:3006:A:N1    | 2.49                     | 0.42              |
| 61:B2:890:U:O4    | 61:B2:891:A:N6     | 2.52                     | 0.42              |
| 61:B2:1123:G:H2'  | 61:B2:1124:C:C6    | 2.55                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 61:B2:1533:C:H2'   | 61:B2:1534:G:C8    | 2.55                     | 0.42              |
| 62:A5:712:U:H2'    | 62:A5:713:U:C6     | 2.55                     | 0.42              |
| 62:A5:1702:G:H2'   | 62:A5:1703:A:C8    | 2.53                     | 0.42              |
| 62:A5:2019:U:H3    | 62:A5:2052:G:N2    | 2.16                     | 0.42              |
| 62:A5:3369:A:O2'   | 62:A5:3382:G:N2    | 2.53                     | 0.42              |
| 66:Cg:39:PRO:HB2   | 66:Cg:56:PRO:HB2   | 2.01                     | 0.42              |
| 69:AT:83:LYS:HZ3   | 69:AT:95:ALA:HA    | 1.83                     | 0.42              |
| 70:AF:92:ILE:O     | 70:AF:96:LEU:N     | 2.49                     | 0.42              |
| 71:CF:150:LEU:HD12 | 71:CF:199:PHE:HE2  | 1.85                     | 0.42              |
| 79:CV:126:ALA:HB1  | 79:CV:133:ALA:HB2  | 2.02                     | 0.42              |
| 1:AA:125:THR:OG1   | 1:AA:126:ASP:N     | 2.53                     | 0.42              |
| 2:CA:1:MET:SD      | 62:A5:1108:G:O2'   | 2.65                     | 0.42              |
| 3:AB:126:ALA:N     | 3:AB:142:CYS:O     | 2.52                     | 0.42              |
| 6:CC:11:SER:N      | 6:CC:152:GLU:OE2   | 2.37                     | 0.42              |
| 6:CC:251:ARG:HH11  | 6:CC:251:ARG:HD3   | 1.73                     | 0.42              |
| 6:CC:312:VAL:HG23  | 6:CC:314:ARG:HG2   | 2.02                     | 0.42              |
| 7:Ag:250:CYS:SG    | 7:Ag:292:TRP:NE1   | 2.76                     | 0.42              |
| 9:AO:22:ARG:HH22   | 9:AO:91:THR:HG21   | 1.84                     | 0.42              |
| 10:AX:24:ASP:HB2   | 61:B2:617:U:C4     | 2.54                     | 0.42              |
| 18:AV:53:TYR:OH    | 18:AV:76:ASP:OD2   | 2.29                     | 0.42              |
| 19:AY:108:ARG:HD3  | 19:AY:108:ARG:HA   | 1.81                     | 0.42              |
| 23:AD:52:ILE:HB    | 23:AD:90:ALA:HA    | 2.02                     | 0.42              |
| 27:Ca:1:MET:N      | 62:A5:1669:G:OP1   | 2.29                     | 0.42              |
| 34:CT:6:GLY:HA3    | 34:CT:7:TYR:HD1    | 1.84                     | 0.42              |
| 34:CT:6:GLY:HA3    | 34:CT:7:TYR:CD1    | 2.54                     | 0.42              |
| 53:CJ:5:THR:HG23   | 58:A7:19:C:H5''    | 2.02                     | 0.42              |
| 53:CJ:25:LEU:HB3   | 53:CJ:79:VAL:HG13  | 2.01                     | 0.42              |
| 58:A7:101:A:H2'    | 58:A7:102:C:H6     | 1.85                     | 0.42              |
| 61:B2:847:G:H21    | 61:B2:850:U:H4'    | 1.84                     | 0.42              |
| 61:B2:1424:A:H1'   | 76:AQ:128:ARG:HH22 | 1.84                     | 0.42              |
| 62:A5:32:C:H4'     | 62:A5:65:A:H2      | 1.83                     | 0.42              |
| 62:A5:230:C:H2'    | 62:A5:231:A:C8     | 2.50                     | 0.42              |
| 62:A5:615:C:H2'    | 62:A5:616:A:C8     | 2.53                     | 0.42              |
| 62:A5:847:A:H2'    | 62:A5:848:A:C8     | 2.54                     | 0.42              |
| 62:A5:1035:G:N2    | 62:A5:1058:A:H62   | 2.17                     | 0.42              |
| 62:A5:2141:A:H2'   | 62:A5:2142:A:H8    | 1.85                     | 0.42              |
| 62:A5:2250:G:N1    | 62:A5:2251:G:N7    | 2.68                     | 0.42              |
| 62:A5:2809:C:H2'   | 62:A5:2810:A:H8    | 1.85                     | 0.42              |
| 62:A5:3831:C:H2'   | 62:A5:3832:A:H8    | 1.85                     | 0.42              |
| 69:AT:19:ALA:O     | 69:AT:23:LYS:CG    | 2.67                     | 0.42              |
| 69:AT:57:CYS:O     | 69:AT:61:LEU:HG    | 2.20                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 75:AI:196:GLU:HA   | 75:AI:199:PHE:HB3  | 2.01                     | 0.42              |
| 80:CM:82:LEU:HA    | 80:CM:85:GLN:HG2   | 2.01                     | 0.42              |
| 80:CM:136:ALA:HA   | 80:CM:137:ASP:HA   | 1.80                     | 0.42              |
| 5:AC:100:ARG:HH12  | 61:B2:1235:A:H5'   | 1.84                     | 0.42              |
| 7:Ag:4:THR:OG1     | 7:Ag:269:GLU:OE1   | 2.37                     | 0.42              |
| 9:AO:34:TYR:HD1    | 9:AO:98:ARG:HB3    | 1.85                     | 0.42              |
| 17:AP:118:TYR:HB2  | 17:AP:121:GLU:HG3  | 2.02                     | 0.42              |
| 24:Ae:111:ASN:O    | 24:Ae:116:ASN:ND2  | 2.46                     | 0.42              |
| 26:AJ:148:PHE:O    | 61:B2:847:G:N2     | 2.43                     | 0.42              |
| 28:CN:173:GLY:O    | 28:CN:183:THR:OG1  | 2.25                     | 0.42              |
| 33:CS:132:ILE:HD11 | 33:CS:136:LYS:HE2  | 2.02                     | 0.42              |
| 35:CP:27:LYS:HG3   | 35:CP:63:PHE:CE2   | 2.55                     | 0.42              |
| 39:Cr:75:GLN:HE21  | 39:Cr:83:ARG:NE    | 2.14                     | 0.42              |
| 44:Ce:91:ASN:HD22  | 44:Ce:91:ASN:N     | 2.17                     | 0.42              |
| 45:Cf:80:ARG:HH12  | 62:A5:1396:A:H62   | 1.67                     | 0.42              |
| 46:Ci:16:LYS:NZ    | 46:Ci:18:SER:O     | 2.36                     | 0.42              |
| 52:Co:34:GLY:O     | 52:Co:39:ARG:NH1   | 2.43                     | 0.42              |
| 52:Co:97:ARG:NH1   | 52:Co:100:GLN:OE1  | 2.53                     | 0.42              |
| 53:CJ:90:ARG:O     | 53:CJ:93:LYS:NZ    | 2.42                     | 0.42              |
| 61:B2:217:A:H62    | 61:B2:915:U:H5     | 1.67                     | 0.42              |
| 61:B2:984:G:H22    | 61:B2:1003:C:N4    | 2.18                     | 0.42              |
| 62:A5:71:A:N7      | 62:A5:319:G:O2'    | 2.49                     | 0.42              |
| 62:A5:626:A:H2'    | 62:A5:627:G:H8     | 1.83                     | 0.42              |
| 62:A5:663:U:N3     | 62:A5:751:A:H5'    | 2.35                     | 0.42              |
| 62:A5:782:G:H8     | 62:A5:782:G:O5'    | 2.03                     | 0.42              |
| 62:A5:1006:A:H62   | 62:A5:1007:A:N6    | 2.17                     | 0.42              |
| 62:A5:1121:A:C2    | 83:Cj:4:GLY:O      | 2.73                     | 0.42              |
| 62:A5:2111:A:H3'   | 62:A5:2112:A:H8    | 1.84                     | 0.42              |
| 62:A5:3577:U:P     | 79:CV:15:ARG:HH21  | 2.43                     | 0.42              |
| 62:A5:3642:G:N1    | 62:A5:3661:C:N3    | 2.68                     | 0.42              |
| 69:AT:54:TYR:CD1   | 69:AT:103:ALA:HB1  | 2.55                     | 0.42              |
| 69:AT:85:ASN:HD22  | 69:AT:91:HIS:HB2   | 1.85                     | 0.42              |
| 72:AE:134:LYS:HA   | 72:AE:135:GLY:HA2  | 1.71                     | 0.42              |
| 72:AE:249:ALA:HB2  | 72:AE:252:ARG:HH21 | 1.85                     | 0.42              |
| 75:AI:67:TRP:CG    | 75:AI:113:TYR:HH   | 2.37                     | 0.42              |
| 77:CO:93:LYS:HB2   | 77:CO:93:LYS:HE2   | 1.83                     | 0.42              |
| 2:CA:104:LEU:HA    | 2:CA:107:MET:HE3   | 2.02                     | 0.42              |
| 2:CA:152:SER:OG    | 2:CA:153:GLY:N     | 2.53                     | 0.42              |
| 3:AB:119:LYS:O     | 3:AB:121:GLN:N     | 2.53                     | 0.42              |
| 3:AB:210:LEU:HD11  | 3:AB:213:VAL:HB    | 2.02                     | 0.42              |
| 4:CB:120:LYS:N     | 62:A5:3870:A:OP1   | 2.53                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:CC:72:THR:HA    | 6:CC:73:GLY:HA2   | 1.49                     | 0.42              |
| 6:CC:123:ARG:NH1  | 62:A5:844:C:OP2   | 2.41                     | 0.42              |
| 10:AX:17:ARG:NH2  | 61:B2:619:U:OP1   | 2.38                     | 0.42              |
| 14:AN:16:LEU:HD23 | 14:AN:16:LEU:HA   | 1.89                     | 0.42              |
| 14:AN:63:VAL:HA   | 14:AN:66:VAL:HG12 | 2.01                     | 0.42              |
| 19:AY:18:LEU:O    | 72:AE:94:LYS:NZ   | 2.52                     | 0.42              |
| 22:Ab:34:ASP:HB3  | 22:Ab:43:ILE:HD11 | 2.01                     | 0.42              |
| 28:CN:68:ARG:NH1  | 28:CN:125:ALA:H   | 2.17                     | 0.42              |
| 33:CS:95:ARG:NH1  | 62:A5:1427:G:O3'  | 2.53                     | 0.42              |
| 35:CP:31:GLU:OE2  | 35:CP:63:PHE:HB2  | 2.20                     | 0.42              |
| 37:CY:124:LYS:O   | 37:CY:128:ALA:N   | 2.42                     | 0.42              |
| 44:Ce:17:LYS:NZ   | 62:A5:775:U:O5'   | 2.44                     | 0.42              |
| 45:Cf:59:TYR:O    | 45:Cf:61:ARG:N    | 2.53                     | 0.42              |
| 46:Ci:45:ARG:H    | 46:Ci:45:ARG:HG3  | 1.68                     | 0.42              |
| 48:Cl:4:HIS:HB3   | 62:A5:1872:A:C2   | 2.55                     | 0.42              |
| 52:Co:65:LYS:HG2  | 52:Co:85:ARG:HG2  | 2.02                     | 0.42              |
| 54:CH:184:THR:OG1 | 54:CH:187:LYS:O   | 2.37                     | 0.42              |
| 55:CE:150:SER:HB2 | 80:CM:107:PHE:CD2 | 2.55                     | 0.42              |
| 61:B2:12:U:H2'    | 61:B2:13:C:C6     | 2.55                     | 0.42              |
| 61:B2:1258:G:H22  | 61:B2:1763:C:HO2' | 1.62                     | 0.42              |
| 61:B2:1425:U:H4'  | 61:B2:1603:G:H1'  | 2.02                     | 0.42              |
| 61:B2:1527:U:H2'  | 61:B2:1528:G:C4   | 2.55                     | 0.42              |
| 62:A5:43:A:N7     | 62:A5:46:C:H5     | 2.18                     | 0.42              |
| 62:A5:403:A:H2'   | 62:A5:404:U:H6    | 1.85                     | 0.42              |
| 62:A5:809:G:N2    | 62:A5:1678:C:N3   | 2.67                     | 0.42              |
| 62:A5:1466:A:C5   | 62:A5:1467:A:H1'  | 2.55                     | 0.42              |
| 62:A5:1950:A:H4'  | 66:Cg:82:HIS:CE1  | 2.55                     | 0.42              |
| 62:A5:2835:G:N2   | 62:A5:2837:A:N7   | 2.68                     | 0.42              |
| 62:A5:3395:G:O2'  | 81:B:75:A:OP1     | 2.26                     | 0.42              |
| 62:A5:3584:C:N4   | 62:A5:3626:A:H62  | 2.18                     | 0.42              |
| 62:A5:3843:U:O3'  | 62:A5:3844:U:H4'  | 2.20                     | 0.42              |
| 72:AE:57:ASN:HD21 | 72:AE:59:ALA:HB3  | 1.84                     | 0.42              |
| 72:AE:179:ASN:ND2 | 72:AE:230:LYS:HD3 | 2.35                     | 0.42              |
| 74:AH:175:TYR:HE2 | 74:AH:181:ARG:HB2 | 1.85                     | 0.42              |
| 76:AQ:13:GLN:HG3  | 76:AQ:26:TYR:HE1  | 1.85                     | 0.42              |
| 2:CA:49:ILE:HD13  | 2:CA:49:ILE:HA    | 1.90                     | 0.41              |
| 2:CA:102:MET:HE2  | 2:CA:107:MET:HE2  | 2.01                     | 0.41              |
| 4:CB:271:GLN:OE1  | 4:CB:272:LYS:N    | 2.53                     | 0.41              |
| 4:CB:283:LYS:NZ   | 4:CB:359:ALA:O    | 2.35                     | 0.41              |
| 4:CB:350:SER:OG   | 4:CB:351:LEU:N    | 2.52                     | 0.41              |
| 7:Ag:46:THR:H     | 7:Ag:54:GLY:HA2   | 1.83                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 8:AU:106:ILE:HA    | 8:AU:107:ASN:HA    | 1.75                     | 0.41              |
| 16:AR:24:LEU:HD21  | 16:AR:34:ILE:HG12  | 2.02                     | 0.41              |
| 20:AZ:56:LYS:HE3   | 20:AZ:56:LYS:HB2   | 1.72                     | 0.41              |
| 20:AZ:90:LEU:HD22  | 20:AZ:95:LEU:HD11  | 2.02                     | 0.41              |
| 22:Ab:23:ARG:NH1   | 74:AH:194:VAL:OXT  | 2.53                     | 0.41              |
| 28:CN:57:GLN:HA    | 28:CN:58:GLY:HA2   | 1.78                     | 0.41              |
| 28:CN:160:GLU:HG2  | 28:CN:161:LEU:HG   | 2.01                     | 0.41              |
| 29:CI:86:HIS:N     | 29:CI:139:ARG:O    | 2.53                     | 0.41              |
| 31:CQ:17:GLU:HB2   | 31:CQ:26:ARG:HH12  | 1.85                     | 0.41              |
| 36:CX:162:ARG:HH11 | 36:CX:163:THR:H    | 1.67                     | 0.41              |
| 36:CX:271:ALA:HB1  | 36:CX:276:ILE:HB   | 2.01                     | 0.41              |
| 37:CY:35:SER:OG    | 37:CY:106:ILE:O    | 2.30                     | 0.41              |
| 42:Cc:29:LEU:HD23  | 42:Cc:29:LEU:HA    | 1.84                     | 0.41              |
| 46:Ci:37:SER:H     | 62:A5:165:G:H5''   | 1.85                     | 0.41              |
| 54:CH:105:GLU:HA   | 54:CH:106:ASN:HA   | 1.77                     | 0.41              |
| 56:CG:252:LEU:HA   | 56:CG:252:LEU:HD12 | 1.94                     | 0.41              |
| 60:Cz:7:ARG:O      | 60:Cz:215:ARG:N    | 2.50                     | 0.41              |
| 61:B2:249:U:N3     | 61:B2:252:A:N7     | 2.68                     | 0.41              |
| 61:B2:496:C:H2'    | 61:B2:497:A:C8     | 2.55                     | 0.41              |
| 61:B2:1075:U:H2'   | 61:B2:1076:U:C6    | 2.55                     | 0.41              |
| 61:B2:1422:A:N1    | 61:B2:1608:U:H1'   | 2.35                     | 0.41              |
| 61:B2:1550:C:O2    | 61:B2:1561:G:N2    | 2.53                     | 0.41              |
| 61:B2:1696:G:H2'   | 69:AT:41:LYS:HZ3   | 1.54                     | 0.41              |
| 62:A5:634:U:H2'    | 62:A5:635:G:H8     | 1.85                     | 0.41              |
| 62:A5:717:A:O2'    | 62:A5:718:U:O4'    | 2.38                     | 0.41              |
| 62:A5:728:U:H2'    | 62:A5:729:G:H8     | 1.85                     | 0.41              |
| 62:A5:783:G:C2     | 62:A5:784:G:C8     | 3.08                     | 0.41              |
| 62:A5:2117:A:H5'   | 66:Cg:70:LYS:HD3   | 2.02                     | 0.41              |
| 62:A5:2807:G:H2'   | 62:A5:2808:G:C8    | 2.55                     | 0.41              |
| 62:A5:3147:A:H2'   | 62:A5:3148:C:H6    | 1.85                     | 0.41              |
| 62:A5:3403:G:H5''  | 62:A5:3404:A:H5'   | 2.02                     | 0.41              |
| 65:CW:2:LYS:HB2    | 65:CW:3:ILE:H      | 1.74                     | 0.41              |
| 71:CF:240:ARG:H    | 71:CF:240:ARG:HG2  | 1.69                     | 0.41              |
| 73:AG:224:LYS:HD3  | 73:AG:224:LYS:HA   | 1.88                     | 0.41              |
| 1:AA:74:ILE:HD11   | 1:AA:123:VAL:HG22  | 2.02                     | 0.41              |
| 2:CA:58:LEU:HD23   | 2:CA:58:LEU:HA     | 1.85                     | 0.41              |
| 3:AB:90:ILE:N      | 3:AB:102:ASN:O     | 2.40                     | 0.41              |
| 4:CB:20:LYS:HB3    | 62:A5:3521:A:H5'   | 2.01                     | 0.41              |
| 4:CB:43:LEU:HD11   | 4:CB:205:ILE:HD13  | 2.01                     | 0.41              |
| 6:CC:104:MET:HE3   | 62:A5:362:A:H5''   | 2.01                     | 0.41              |
| 15:AL:16:ASN:OD1   | 15:AL:18:ASN:OD1   | 2.38                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 17:AP:100:TYR:HD1  | 17:AP:105:PHE:HB2  | 1.85                     | 0.41              |
| 21:Aa:23:CYS:HB3   | 21:Aa:27:ALA:H     | 1.84                     | 0.41              |
| 23:AD:26:PHE:HA    | 23:AD:29:ARG:HB2   | 2.01                     | 0.41              |
| 26:AJ:175:LYS:HD2  | 26:AJ:178:ASN:HB2  | 2.01                     | 0.41              |
| 28:CN:6:TYR:HE2    | 46:Ci:53:LEU:HD21  | 1.86                     | 0.41              |
| 28:CN:11:TYR:HD1   | 28:CN:11:TYR:HA    | 1.66                     | 0.41              |
| 28:CN:23:LEU:HD12  | 28:CN:23:LEU:HA    | 1.87                     | 0.41              |
| 28:CN:199:HIS:HB3  | 78:CL:24:TRP:CD1   | 2.55                     | 0.41              |
| 29:CI:217:TYR:OH   | 30:CD:297:THR:OG1  | 2.28                     | 0.41              |
| 30:CD:236:LEU:HA   | 30:CD:239:ILE:HD12 | 2.02                     | 0.41              |
| 34:CT:14:MET:SD    | 34:CT:58:HIS:ND1   | 2.91                     | 0.41              |
| 39:Cr:116:ARG:HH21 | 44:Ce:89:MET:HE1   | 1.86                     | 0.41              |
| 60:Cz:35:GLN:HA    | 60:Cz:165:LEU:HD23 | 2.02                     | 0.41              |
| 60:Cz:110:PHE:O    | 60:Cz:141:GLN:NE2  | 2.53                     | 0.41              |
| 61:B2:121:A:O2'    | 72:AE:77:ARG:NH2   | 2.48                     | 0.41              |
| 61:B2:957:A:H3'    | 61:B2:958:G:H4'    | 2.02                     | 0.41              |
| 61:B2:1128:C:H2'   | 61:B2:1129:A:C8    | 2.55                     | 0.41              |
| 61:B2:1238:G:N1    | 61:B2:1963:G:N3    | 2.68                     | 0.41              |
| 61:B2:1296:A:O2'   | 61:B2:1624:U:O4    | 2.39                     | 0.41              |
| 61:B2:1884:G:H22   | 61:B2:1903:G:H1'   | 1.85                     | 0.41              |
| 62:A5:270:G:H2'    | 62:A5:271:A:H8     | 1.84                     | 0.41              |
| 62:A5:706:G:N2     | 62:A5:731:U:O2     | 2.52                     | 0.41              |
| 62:A5:1208:U:H2'   | 62:A5:1209:A:H8    | 1.84                     | 0.41              |
| 62:A5:3170:U:O4    | 62:A5:3171:A:N6    | 2.53                     | 0.41              |
| 62:A5:3949:U:O2'   | 62:A5:3952:C:H5''  | 2.20                     | 0.41              |
| 69:AT:63:HIS:HE1   | 69:AT:67:ARG:NH2   | 2.18                     | 0.41              |
| 80:CM:109:ARG:HA   | 80:CM:112:LEU:HB2  | 2.02                     | 0.41              |
| 81:B:9:G:H5'       | 81:B:45:G:H21      | 1.85                     | 0.41              |
| 1:AA:6:ASP:HB2     | 1:AA:7:ILE:H       | 1.75                     | 0.41              |
| 1:AA:84:GLN:HG2    | 1:AA:100:ALA:HB1   | 2.02                     | 0.41              |
| 2:CA:210:PRO:HB2   | 2:CA:211:HIS:CD2   | 2.54                     | 0.41              |
| 3:AB:65:ARG:NH2    | 9:AO:51:GLU:OE1    | 2.53                     | 0.41              |
| 4:CB:328:ASN:OD1   | 4:CB:328:ASN:N     | 2.34                     | 0.41              |
| 6:CC:21:LYS:HA     | 6:CC:21:LYS:HD2    | 1.81                     | 0.41              |
| 9:AO:142:ARG:NH2   | 21:Aa:23:CYS:O     | 2.52                     | 0.41              |
| 10:AX:68:LYS:HB3   | 10:AX:91:LEU:HD11  | 2.01                     | 0.41              |
| 17:AP:25:LEU:HA    | 17:AP:28:LEU:HG    | 2.02                     | 0.41              |
| 27:Ca:37:GLY:O     | 27:Ca:40:HIS:N     | 2.50                     | 0.41              |
| 30:CD:33:ARG:HA    | 30:CD:36:LEU:HB3   | 2.02                     | 0.41              |
| 33:CS:13:VAL:HG22  | 33:CS:29:LYS:HG3   | 2.02                     | 0.41              |
| 35:CP:25:HIS:HB2   | 35:CP:28:ASN:HB2   | 2.02                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 38:CZ:63:LYS:HA   | 38:CZ:63:LYS:HD2   | 1.75                     | 0.41              |
| 39:Cr:35:ASN:C    | 39:Cr:35:ASN:HD22  | 2.28                     | 0.41              |
| 41:Cb:21:ILE:HA   | 41:Cb:21:ILE:HD12  | 1.81                     | 0.41              |
| 43:Cd:37:LYS:O    | 43:Cd:41:ARG:N     | 2.51                     | 0.41              |
| 45:Cf:83:HIS:HD2  | 55:CE:239:HIS:CG   | 2.38                     | 0.41              |
| 53:CJ:149:ARG:NH1 | 58:A7:28:U:OP1     | 2.53                     | 0.41              |
| 57:A9:21:G:H2'    | 57:A9:22:A:H8      | 1.86                     | 0.41              |
| 57:A9:26:U:H3     | 62:A5:10:A:H61     | 1.67                     | 0.41              |
| 61:B2:92:A:H62    | 61:B2:401:G:N2     | 2.18                     | 0.41              |
| 61:B2:353:U:H2'   | 61:B2:354:U:C6     | 2.54                     | 0.41              |
| 61:B2:614:A:H4'   | 61:B2:615:G:H3'    | 2.02                     | 0.41              |
| 61:B2:838:A:H3'   | 61:B2:839:A:H8     | 1.85                     | 0.41              |
| 61:B2:994:A:HO2'  | 61:B2:1084:G:HO2'  | 1.60                     | 0.41              |
| 61:B2:1379:G:N7   | 61:B2:1409:A:N6    | 2.56                     | 0.41              |
| 61:B2:1833:C:N4   | 61:B2:1834:G:O6    | 2.53                     | 0.41              |
| 61:B2:1953:U:H2'  | 61:B2:1954:C:H6    | 1.85                     | 0.41              |
| 62:A5:35:C:H5'    | 62:A5:36:U:OP2     | 2.21                     | 0.41              |
| 62:A5:757:A:O2'   | 62:A5:3842:A:OP2   | 2.38                     | 0.41              |
| 62:A5:1121:A:H4'  | 83:Cj:3:LYS:HB2    | 2.02                     | 0.41              |
| 62:A5:1796:A:N6   | 62:A5:2553:U:OP1   | 2.53                     | 0.41              |
| 62:A5:1931:C:N4   | 62:A5:1935:G:OP2   | 2.52                     | 0.41              |
| 62:A5:1990:G:O3'  | 67:CU:273:ARG:NH2  | 2.52                     | 0.41              |
| 62:A5:2108:U:H4'  | 62:A5:2109:G:H5'   | 2.01                     | 0.41              |
| 62:A5:2652:U:H2'  | 62:A5:2653:A:H8    | 1.84                     | 0.41              |
| 62:A5:3275:G:H2'  | 62:A5:3276:C:C6    | 2.55                     | 0.41              |
| 62:A5:3492:G:H2'  | 62:A5:3493:U:H6    | 1.84                     | 0.41              |
| 62:A5:3558:U:H2'  | 62:A5:3559:A:H8    | 1.85                     | 0.41              |
| 62:A5:3720:A:N7   | 77:CO:118:ARG:NH2  | 2.50                     | 0.41              |
| 70:AF:199:ASP:O   | 70:AF:203:ASN:OD1  | 2.38                     | 0.41              |
| 73:AG:1:MET:HE3   | 73:AG:24:LEU:HD22  | 2.03                     | 0.41              |
| 2:CA:120:THR:HG23 | 2:CA:162:ASN:HA    | 2.01                     | 0.41              |
| 3:AB:222:LYS:HD3  | 3:AB:222:LYS:HA    | 1.72                     | 0.41              |
| 4:CB:117:ARG:HD2  | 4:CB:117:ARG:HA    | 1.72                     | 0.41              |
| 5:AC:101:ALA:HA   | 5:AC:102:GLY:HA2   | 1.71                     | 0.41              |
| 6:CC:58:SER:O     | 6:CC:60:LEU:N      | 2.53                     | 0.41              |
| 6:CC:89:ARG:HD2   | 6:CC:89:ARG:HA     | 1.87                     | 0.41              |
| 6:CC:112:ARG:C    | 28:CN:204:ARG:HH22 | 2.28                     | 0.41              |
| 10:AX:7:LEU:HA    | 15:AL:98:ARG:HE    | 1.86                     | 0.41              |
| 12:AS:86:ARG:HD3  | 12:AS:86:ARG:HA    | 1.85                     | 0.41              |
| 13:Ad:18:SER:HA   | 13:Ad:27:ARG:HH12  | 1.84                     | 0.41              |
| 26:AJ:85:ILE:HA   | 26:AJ:151:ARG:HA   | 2.01                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 35:CP:168:LYS:NZ  | 62:A5:760:G:OP1    | 2.44                     | 0.41              |
| 35:CP:174:LYS:HD2 | 45:Cf:109:GLU:HB3  | 2.03                     | 0.41              |
| 39:Cr:71:GLY:HA3  | 39:Cr:84:VAL:HA    | 2.02                     | 0.41              |
| 41:Cb:45:TYR:CG   | 62:A5:1288:U:H2'   | 2.55                     | 0.41              |
| 47:Ck:51:GLU:OE1  | 47:Ck:55:LYS:NZ    | 2.43                     | 0.41              |
| 49:Cm:98:LYS:HD2  | 49:Cm:118:THR:HG21 | 2.02                     | 0.41              |
| 49:Cm:104:HIS:CD2 | 49:Cm:106:ARG:H    | 2.38                     | 0.41              |
| 53:CJ:5:THR:HA    | 58:A7:19:C:H4'     | 2.01                     | 0.41              |
| 53:CJ:30:CYS:SG   | 62:A5:3207:C:N4    | 2.93                     | 0.41              |
| 60:Cz:35:GLN:HG2  | 60:Cz:205:HIS:HB2  | 2.02                     | 0.41              |
| 61:B2:1262:C:H2'  | 61:B2:1263:U:C6    | 2.56                     | 0.41              |
| 62:A5:72:C:H42    | 62:A5:79:G:H1      | 1.68                     | 0.41              |
| 62:A5:673:U:O2    | 62:A5:750:G:N2     | 2.39                     | 0.41              |
| 62:A5:748:A:O3'   | 62:A5:752:U:N3     | 2.53                     | 0.41              |
| 62:A5:1043:G:H2'  | 62:A5:1044:G:H8    | 1.85                     | 0.41              |
| 62:A5:1499:C:O5'  | 62:A5:1500:G:N2    | 2.54                     | 0.41              |
| 62:A5:1590:A:H2'  | 62:A5:1591:U:C6    | 2.55                     | 0.41              |
| 62:A5:1665:C:H2'  | 62:A5:1666:A:H8    | 1.84                     | 0.41              |
| 62:A5:1789:A:H2'  | 62:A5:1790:A:C8    | 2.55                     | 0.41              |
| 62:A5:2260:U:H2'  | 62:A5:2261:G:H8    | 1.85                     | 0.41              |
| 62:A5:2535:U:O2'  | 62:A5:2536:G:H5'   | 2.20                     | 0.41              |
| 62:A5:2755:G:O2'  | 62:A5:2756:C:O5'   | 2.31                     | 0.41              |
| 62:A5:3197:U:H3   | 62:A5:3236:A:H2    | 1.69                     | 0.41              |
| 62:A5:3638:U:H2'  | 62:A5:3662:G:N2    | 2.35                     | 0.41              |
| 62:A5:3808:A:O2'  | 62:A5:3809:U:OP2   | 2.35                     | 0.41              |
| 63:Ac:30:PHE:HE1  | 63:Ac:54:LEU:HD23  | 1.86                     | 0.41              |
| 69:AT:50:PRO:CA   | 69:AT:53:PHE:HD2   | 2.32                     | 0.41              |
| 70:AF:139:ALA:O   | 70:AF:143:SER:OG   | 2.29                     | 0.41              |
| 70:AF:180:THR:OG1 | 70:AF:181:GLY:N    | 2.51                     | 0.41              |
| 71:CF:35:GLU:H    | 71:CF:35:GLU:HG2   | 1.75                     | 0.41              |
| 79:CV:82:ILE:HB   | 79:CV:121:VAL:HG12 | 2.03                     | 0.41              |
| 1:AA:200:ASP:OD1  | 1:AA:200:ASP:N     | 2.53                     | 0.41              |
| 5:AC:165:CYS:HB2  | 64:AW:95:PRO:HB2   | 2.02                     | 0.41              |
| 9:AO:146:ARG:NH1  | 21:Aa:29:CYS:SG    | 2.94                     | 0.41              |
| 19:AY:17:ARG:O    | 72:AE:94:LYS:NZ    | 2.37                     | 0.41              |
| 23:AD:179:LEU:HB3 | 23:AD:183:VAL:N    | 2.36                     | 0.41              |
| 23:AD:203:LYS:HB3 | 23:AD:205:PRO:HD3  | 2.03                     | 0.41              |
| 29:CI:63:GLU:OE1  | 29:CI:63:GLU:N     | 2.54                     | 0.41              |
| 33:CS:157:ARG:HG3 | 62:A5:3753:A:H8    | 1.83                     | 0.41              |
| 33:CS:170:ARG:NH1 | 62:A5:3761:U:O4    | 2.53                     | 0.41              |
| 35:CP:174:LYS:HZ3 | 35:CP:178:GLN:NE2  | 2.18                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 51:Cp:24:LYS:HE2   | 51:Cp:28:LYS:HE2   | 2.01                     | 0.41              |
| 58:A7:5:A:H61      | 58:A7:114:U:H3     | 1.68                     | 0.41              |
| 61:B2:62:A:H1'     | 61:B2:274:G:H1'    | 2.03                     | 0.41              |
| 61:B2:97:U:H3      | 61:B2:390:A:H61    | 1.69                     | 0.41              |
| 62:A5:80:G:N1      | 62:A5:333:C:OP1    | 2.46                     | 0.41              |
| 62:A5:190:A:H1'    | 62:A5:191:A:C8     | 2.55                     | 0.41              |
| 62:A5:766:G:H3'    | 62:A5:767:A:C8     | 2.55                     | 0.41              |
| 62:A5:1209:A:H61   | 62:A5:1266:A:H1'   | 1.86                     | 0.41              |
| 62:A5:1764:G:N2    | 62:A5:1765:U:O4    | 2.53                     | 0.41              |
| 62:A5:2064:G:H1    | 62:A5:2082:U:P     | 2.44                     | 0.41              |
| 62:A5:3216:C:H2'   | 62:A5:3217:A:C8    | 2.56                     | 0.41              |
| 62:A5:3499:G:H2'   | 62:A5:3500:A:H8    | 1.86                     | 0.41              |
| 69:AT:30:VAL:HG13  | 69:AT:31:PRO:HD3   | 2.02                     | 0.41              |
| 69:AT:59:SER:O     | 69:AT:63:HIS:N     | 2.49                     | 0.41              |
| 72:AE:73:ASP:HB3   | 72:AE:164:ILE:HG21 | 2.01                     | 0.41              |
| 72:AE:207:ILE:HG22 | 72:AE:221:ARG:HA   | 2.02                     | 0.41              |
| 73:AG:50:LEU:HA    | 73:AG:113:VAL:HA   | 2.03                     | 0.41              |
| 74:AH:56:LYS:HB2   | 74:AH:88:LYS:HG2   | 2.03                     | 0.41              |
| 83:Cj:65:ARG:HG3   | 83:Cj:65:ARG:HH11  | 1.85                     | 0.41              |
| 6:CC:287:MET:SD    | 31:CQ:27:LEU:HB3   | 2.61                     | 0.41              |
| 6:CC:389:LYS:HE2   | 6:CC:389:LYS:HB3   | 1.82                     | 0.41              |
| 8:AU:76:SER:O      | 8:AU:78:THR:N      | 2.54                     | 0.41              |
| 10:AX:88:ASP:OD1   | 10:AX:88:ASP:N     | 2.53                     | 0.41              |
| 11:AM:87:ASP:OD1   | 11:AM:87:ASP:N     | 2.53                     | 0.41              |
| 12:AS:84:LEU:HD23  | 12:AS:84:LEU:HA    | 1.80                     | 0.41              |
| 12:AS:129:LEU:HG   | 12:AS:136:THR:HG21 | 2.01                     | 0.41              |
| 16:AR:52:GLY:O     | 16:AR:56:HIS:ND1   | 2.35                     | 0.41              |
| 20:AZ:97:LYS:N     | 20:AZ:109:THR:O    | 2.39                     | 0.41              |
| 23:AD:140:VAL:HG12 | 23:AD:154:PHE:HE2  | 1.86                     | 0.41              |
| 26:AJ:13:THR:N     | 61:B2:477:A:OP1    | 2.52                     | 0.41              |
| 38:CZ:4:ILE:HG23   | 38:CZ:5:MET:HG2    | 2.01                     | 0.41              |
| 38:CZ:53:VAL:HG13  | 38:CZ:57:MET:HE2   | 2.02                     | 0.41              |
| 39:Cr:126:LYS:HD2  | 39:Cr:127:PRO:HA   | 2.02                     | 0.41              |
| 45:Cf:94:TYR:CD1   | 45:Cf:148:ILE:HG22 | 2.56                     | 0.41              |
| 45:Cf:123:ARG:NH2  | 62:A5:1381:U:OP1   | 2.41                     | 0.41              |
| 46:Ci:9:ILE:HD13   | 46:Ci:9:ILE:HA     | 1.96                     | 0.41              |
| 48:Cl:21:ARG:HH11  | 48:Cl:21:ARG:HD2   | 1.73                     | 0.41              |
| 55:CE:89:ARG:H     | 55:CE:89:ARG:HG2   | 1.66                     | 0.41              |
| 56:CG:63:PRO:HB2   | 56:CG:66:ILE:HG12  | 2.02                     | 0.41              |
| 57:A9:15:A:N6      | 62:A5:21:U:H3      | 2.17                     | 0.41              |
| 60:Cz:41:TYR:OH    | 60:Cz:195:LYS:O    | 2.29                     | 0.41              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 61:B2:15:U:O2'     | 61:B2:627:A:N7    | 2.51                     | 0.41              |
| 61:B2:179:A:H3'    | 61:B2:180:A:C8    | 2.56                     | 0.41              |
| 61:B2:390:A:N6     | 61:B2:391:G:O6    | 2.54                     | 0.41              |
| 61:B2:598:C:H2'    | 61:B2:599:A:H8    | 1.84                     | 0.41              |
| 61:B2:603:G:H2'    | 61:B2:604:C:C6    | 2.56                     | 0.41              |
| 61:B2:610:U:H2'    | 61:B2:611:U:C6    | 2.54                     | 0.41              |
| 61:B2:1728:G:C6    | 61:B2:1730:U:H1'  | 2.56                     | 0.41              |
| 61:B2:1799:A:H2'   | 61:B2:1800:U:C6   | 2.56                     | 0.41              |
| 62:A5:795:A:C4     | 62:A5:2750:A:C6   | 3.08                     | 0.41              |
| 62:A5:836:G:OP2    | 78:CL:38:ARG:NH2  | 2.52                     | 0.41              |
| 62:A5:1324:C:H4'   | 62:A5:1325:C:H5'  | 2.01                     | 0.41              |
| 62:A5:1515:U:H3'   | 62:A5:1516:A:H2'  | 2.02                     | 0.41              |
| 62:A5:1902:U:H3    | 62:A5:2142:A:H61  | 1.69                     | 0.41              |
| 62:A5:2771:G:H22   | 62:A5:3516:C:H42  | 1.68                     | 0.41              |
| 62:A5:3499:G:H2'   | 62:A5:3500:A:C8   | 2.55                     | 0.41              |
| 65:CW:56:ARG:HA    | 65:CW:56:ARG:HD3  | 1.80                     | 0.41              |
| 69:AT:19:ALA:O     | 69:AT:23:LYS:HD2  | 2.19                     | 0.41              |
| 77:CO:4:LEU:HD13   | 77:CO:34:LYS:HE3  | 2.02                     | 0.41              |
| 77:CO:22:ALA:O     | 77:CO:26:ALA:N    | 2.40                     | 0.41              |
| 83:Cj:26:SER:HB2   | 83:Cj:35:SER:HB2  | 2.02                     | 0.41              |
| 1:AA:111:GLN:HG3   | 61:B2:1411:G:N3   | 2.36                     | 0.41              |
| 2:CA:51:ASP:HB2    | 2:CA:58:LEU:HG    | 2.02                     | 0.41              |
| 3:AB:91:ALA:HA     | 3:AB:101:CYS:HA   | 2.03                     | 0.41              |
| 4:CB:87:VAL:O      | 4:CB:107:ALA:N    | 2.42                     | 0.41              |
| 4:CB:141:LEU:O     | 4:CB:145:SER:OG   | 2.32                     | 0.41              |
| 5:AC:253:SER:HA    | 5:AC:256:LEU:HB3  | 2.03                     | 0.41              |
| 6:CC:155:LEU:HD21  | 6:CC:177:LEU:HD13 | 2.03                     | 0.41              |
| 12:AS:108:ARG:O    | 12:AS:112:GLU:N   | 2.47                     | 0.41              |
| 14:AN:85:PRO:HD2   | 14:AN:88:LEU:HD11 | 2.03                     | 0.41              |
| 24:Ae:83:LYS:NZ    | 24:Ae:87:GLN:OE1  | 2.51                     | 0.41              |
| 28:CN:18:VAL:HA    | 56:CG:82:PRO:HG3  | 2.02                     | 0.41              |
| 28:CN:96:ARG:NH1   | 28:CN:100:SER:OG  | 2.54                     | 0.41              |
| 29:CI:171:TRP:HB2  | 29:CI:178:ARG:HA  | 2.01                     | 0.41              |
| 31:CQ:174:PHE:HZ   | 62:A5:91:U:H5'    | 1.86                     | 0.41              |
| 33:CS:42:SER:HA    | 33:CS:45:TRP:HD1  | 1.86                     | 0.41              |
| 33:CS:93:MET:HE1   | 62:A5:1428:G:H4'  | 2.02                     | 0.41              |
| 36:CX:161:ILE:HG21 | 56:CG:55:ASP:HA   | 2.03                     | 0.41              |
| 42:Cc:20:LEU:O     | 42:Cc:24:SER:OG   | 2.32                     | 0.41              |
| 54:CH:1:MET:HE3    | 54:CH:1:MET:HB2   | 1.86                     | 0.41              |
| 56:CG:248:GLY:HA2  | 56:CG:249:SER:HA  | 1.73                     | 0.41              |
| 58:A7:11:A:H4'     | 58:A7:13:A:C5     | 2.56                     | 0.41              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 61:B2:244:A:N6     | 61:B2:917:U:OP2   | 2.53                     | 0.41              |
| 61:B2:280:U:O2'    | 61:B2:282:U:O4    | 2.39                     | 0.41              |
| 61:B2:490:A:H2'    | 61:B2:491:G:H8    | 1.86                     | 0.41              |
| 61:B2:1143:A:N7    | 61:B2:1144:C:N4   | 2.68                     | 0.41              |
| 61:B2:1460:A:OP2   | 61:B2:1528:G:N2   | 2.53                     | 0.41              |
| 61:B2:1783:U:H3    | 61:B2:1797:G:H22  | 1.68                     | 0.41              |
| 62:A5:68:G:C6      | 62:A5:340:U:H5    | 2.38                     | 0.41              |
| 62:A5:684:A:H2'    | 62:A5:685:A:C4    | 2.55                     | 0.41              |
| 62:A5:1273:U:H2'   | 62:A5:1274:A:C8   | 2.53                     | 0.41              |
| 62:A5:1914:U:H3    | 62:A5:1921:U:H3   | 1.68                     | 0.41              |
| 62:A5:2205:G:H2'   | 62:A5:2206:U:H6   | 1.86                     | 0.41              |
| 62:A5:2238:A:H62   | 62:A5:2245:G:H21  | 1.69                     | 0.41              |
| 62:A5:2239:C:H42   | 62:A5:2245:G:N2   | 2.19                     | 0.41              |
| 62:A5:2263:A:N6    | 62:A5:2472:A:H61  | 2.19                     | 0.41              |
| 62:A5:2575:C:H42   | 62:A5:2622:A:H62  | 1.68                     | 0.41              |
| 62:A5:2809:C:H42   | 62:A5:3130:G:H1   | 1.68                     | 0.41              |
| 69:AT:29:LYS:HD3   | 69:AT:105:GLN:C   | 2.44                     | 0.41              |
| 71:CF:49:ARG:HA    | 71:CF:52:GLU:HB2  | 2.02                     | 0.41              |
| 73:AG:25:ARG:HA    | 73:AG:28:TYR:HB2  | 2.01                     | 0.41              |
| 75:AI:113:TYR:O    | 75:AI:117:TYR:N   | 2.48                     | 0.41              |
| 79:CV:52:LEU:HD23  | 79:CV:52:LEU:HA   | 1.92                     | 0.41              |
| 83:Cj:37:CYS:HB2   | 83:Cj:38:GLY:H    | 1.59                     | 0.41              |
| 83:Cj:51:ARG:HA    | 83:Cj:51:ARG:HD3  | 1.90                     | 0.41              |
| 3:AB:125:GLU:OE1   | 3:AB:168:ARG:NH1  | 2.54                     | 0.41              |
| 4:CB:268:ARG:HA    | 4:CB:268:ARG:HD2  | 1.69                     | 0.41              |
| 6:CC:198:THR:HG22  | 6:CC:203:ARG:HD2  | 2.03                     | 0.41              |
| 7:Ag:82:GLY:HA2    | 7:Ag:88:LEU:HA    | 2.03                     | 0.41              |
| 7:Ag:193:ASN:ND2   | 23:AD:221:TYR:O   | 2.48                     | 0.41              |
| 9:AO:75:MET:HB3    | 9:AO:75:MET:HE3   | 1.74                     | 0.41              |
| 12:AS:120:HIS:H    | 17:AP:121:GLU:HB3 | 1.85                     | 0.41              |
| 18:AV:42:GLU:HG2   | 18:AV:43:THR:H    | 1.85                     | 0.41              |
| 21:Aa:7:ASN:OD1    | 21:Aa:7:ASN:N     | 2.54                     | 0.41              |
| 21:Aa:64:LEU:HA    | 21:Aa:65:PRO:HD3  | 1.94                     | 0.41              |
| 24:Ae:126:GLY:HA2  | 24:Ae:127:PRO:HD3 | 1.92                     | 0.41              |
| 27:Ca:110:TYR:CD2  | 27:Ca:128:LYS:HD3 | 2.55                     | 0.41              |
| 29:CI:152:LEU:HD23 | 29:CI:152:LEU:HA  | 1.95                     | 0.41              |
| 30:CD:184:SER:O    | 30:CD:184:SER:OG  | 2.38                     | 0.41              |
| 30:CD:209:ARG:HA   | 30:CD:212:GLU:HB2 | 2.02                     | 0.41              |
| 33:CS:111:ARG:HB3  | 62:A5:1537:G:H21  | 1.85                     | 0.41              |
| 39:Cr:108:LYS:H    | 62:A5:1566:U:H5'  | 1.85                     | 0.41              |
| 41:Cb:64:ILE:HD12  | 41:Cb:70:LYS:HZ3  | 1.86                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 42:Cc:33:GLN:N     | 62:A5:2043:G:O6    | 2.53                     | 0.41              |
| 52:Co:52:THR:H     | 52:Co:52:THR:HG23  | 1.63                     | 0.41              |
| 56:CG:128:LYS:HA   | 56:CG:130:LYS:HE2  | 2.03                     | 0.41              |
| 58:A7:30:G:N1      | 58:A7:48:G:N7      | 2.69                     | 0.41              |
| 61:B2:490:A:H2'    | 61:B2:491:G:C8     | 2.56                     | 0.41              |
| 61:B2:1043:U:H1'   | 61:B2:1134:G:H1'   | 2.02                     | 0.41              |
| 61:B2:1312:G:H22   | 61:B2:1345:U:H4'   | 1.86                     | 0.41              |
| 61:B2:1438:U:N3    | 61:B2:1568:G:N3    | 2.68                     | 0.41              |
| 61:B2:1446:G:H1    | 61:B2:1539:U:H1'   | 1.85                     | 0.41              |
| 62:A5:737:U:O4     | 62:A5:738:A:N6     | 2.50                     | 0.41              |
| 62:A5:1292:G:H1'   | 62:A5:1296:U:C4    | 2.55                     | 0.41              |
| 62:A5:1559:A:H2'   | 62:A5:1560:A:C8    | 2.55                     | 0.41              |
| 62:A5:1988:A:H62   | 62:A5:2004:G:H21   | 1.68                     | 0.41              |
| 62:A5:2207:A:H2'   | 62:A5:2208:G:H8    | 1.86                     | 0.41              |
| 62:A5:3364:C:H4'   | 62:A5:3419:A:C8    | 2.56                     | 0.41              |
| 62:A5:3470:G:H2'   | 62:A5:3471:A:C8    | 2.55                     | 0.41              |
| 68:AK:15:LEU:HA    | 68:AK:18:GLU:HB2   | 2.02                     | 0.41              |
| 75:AI:84:ASN:HD22  | 75:AI:90:LEU:HB2   | 1.86                     | 0.41              |
| 75:AI:121:LEU:HA   | 75:AI:122:GLY:HA2  | 1.75                     | 0.41              |
| 77:CO:180:THR:O    | 77:CO:184:ARG:N    | 2.53                     | 0.41              |
| 79:CV:91:ARG:HD3   | 79:CV:91:ARG:HA    | 1.85                     | 0.41              |
| 2:CA:1:MET:N       | 62:A5:2793:C:OP2   | 2.38                     | 0.41              |
| 2:CA:32:LEU:HD12   | 2:CA:121:GLY:HA2   | 2.02                     | 0.41              |
| 2:CA:41:ILE:HD12   | 2:CA:41:ILE:HA     | 1.88                     | 0.41              |
| 2:CA:65:ASP:CG     | 2:CA:67:TYR:H      | 2.28                     | 0.41              |
| 2:CA:219:ILE:O     | 2:CA:221:LYS:N     | 2.54                     | 0.41              |
| 3:AB:201:GLU:HA    | 3:AB:210:LEU:HD23  | 2.03                     | 0.41              |
| 4:CB:53:MET:HE2    | 4:CB:53:MET:HB3    | 1.85                     | 0.41              |
| 5:AC:153:TRP:HZ3   | 5:AC:161:HIS:HB2   | 1.86                     | 0.41              |
| 6:CC:116:ARG:HH11  | 6:CC:118:VAL:HG12  | 1.84                     | 0.41              |
| 6:CC:168:LYS:HE2   | 6:CC:168:LYS:HB3   | 1.71                     | 0.41              |
| 7:Ag:99:THR:OG1    | 7:Ag:100:ARG:N     | 2.54                     | 0.41              |
| 7:Ag:146:ASP:OD2   | 7:Ag:176:LYS:NZ    | 2.54                     | 0.41              |
| 8:AU:51:ARG:HH22   | 61:B2:1558:A:H1'   | 1.85                     | 0.41              |
| 10:AX:3:LYS:HD2    | 61:B2:619:U:H5'    | 2.02                     | 0.41              |
| 11:AM:42:ILE:HG22  | 11:AM:115:VAL:HB   | 2.03                     | 0.41              |
| 12:AS:104:ASP:N    | 12:AS:104:ASP:OD1  | 2.52                     | 0.41              |
| 12:AS:111:LEU:HD13 | 12:AS:114:LEU:HD23 | 2.03                     | 0.41              |
| 18:AV:57:GLY:HA2   | 18:AV:60:ARG:HB2   | 2.03                     | 0.41              |
| 26:AJ:4:GLY:HA3    | 26:AJ:5:ARG:HA     | 1.69                     | 0.41              |
| 26:AJ:30:LEU:HD12  | 26:AJ:31:LYS:HD2   | 2.02                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 26:AJ:114:GLN:HA   | 26:AJ:117:LYS:HG2  | 2.01                     | 0.41              |
| 26:AJ:134:ARG:HH11 | 61:B2:522:G:H5''   | 1.86                     | 0.41              |
| 28:CN:66:VAL:HG12  | 28:CN:67:ARG:H     | 1.84                     | 0.41              |
| 29:CI:35:ASP:OD1   | 29:CI:35:ASP:N     | 2.54                     | 0.41              |
| 30:CD:53:VAL:HG22  | 30:CD:62:VAL:HG22  | 2.02                     | 0.41              |
| 31:CQ:42:LYS:HG3   | 31:CQ:46:ILE:HD11  | 2.02                     | 0.41              |
| 32:CR:21:LYS:HZ3   | 62:A5:2189:U:P     | 2.44                     | 0.41              |
| 34:CT:7:TYR:HB3    | 34:CT:54:TYR:CE2   | 2.56                     | 0.41              |
| 36:CX:182:PRO:HB2  | 36:CX:185:SER:HB3  | 2.03                     | 0.41              |
| 36:CX:191:ARG:HD3  | 59:A8:58:C:C2      | 2.55                     | 0.41              |
| 36:CX:248:LEU:HD21 | 36:CX:256:LYS:HE2  | 2.03                     | 0.41              |
| 38:CZ:134:ARG:HD2  | 38:CZ:134:ARG:HA   | 1.81                     | 0.41              |
| 39:Cr:47:ILE:H     | 39:Cr:47:ILE:HG13  | 1.58                     | 0.41              |
| 40:Ch:44:LEU:HD23  | 40:Ch:44:LEU:HA    | 1.98                     | 0.41              |
| 41:Cb:38:LYS:HA    | 41:Cb:40:LEU:N     | 2.35                     | 0.41              |
| 43:Cd:26:LEU:HD21  | 43:Cd:42:ALA:HB1   | 2.03                     | 0.41              |
| 44:Ce:66:ARG:HD3   | 44:Ce:66:ARG:HA    | 1.85                     | 0.41              |
| 44:Ce:91:ASN:HB2   | 44:Ce:119:VAL:HG12 | 2.03                     | 0.41              |
| 44:Ce:106:LYS:HB3  | 44:Ce:106:LYS:HE3  | 1.83                     | 0.41              |
| 45:Cf:31:LYS:H     | 45:Cf:31:LYS:HG3   | 1.70                     | 0.41              |
| 45:Cf:123:ARG:HH12 | 62:A5:1381:U:P     | 2.42                     | 0.41              |
| 46:Ci:43:GLN:OE1   | 46:Ci:48:LYS:N     | 2.54                     | 0.41              |
| 46:Ci:65:LYS:HA    | 46:Ci:68:MET:HE3   | 2.03                     | 0.41              |
| 53:CJ:24:LYS:HZ1   | 62:A5:3215:A:H5''  | 1.86                     | 0.41              |
| 55:CE:87:HIS:HA    | 62:A5:755:A:C6     | 2.56                     | 0.41              |
| 55:CE:108:HIS:HB3  | 55:CE:111:LYS:HD2  | 2.03                     | 0.41              |
| 55:CE:116:LEU:HD11 | 55:CE:127:THR:HG22 | 2.02                     | 0.41              |
| 56:CG:201:ARG:NH1  | 56:CG:204:CYS:SG   | 2.94                     | 0.41              |
| 56:CG:214:ASN:HA   | 56:CG:217:LYS:HB2  | 2.02                     | 0.41              |
| 58:A7:104:C:P      | 62:A5:1214:G:H22   | 2.43                     | 0.41              |
| 58:A7:105:C:H2'    | 58:A7:106:G:C8     | 2.56                     | 0.41              |
| 60:Cz:128:LEU:O    | 60:Cz:132:GLY:N    | 2.49                     | 0.41              |
| 61:B2:1251:A:H4'   | 70:AF:169:ARG:HH12 | 1.86                     | 0.41              |
| 61:B2:1274:U:OP1   | 61:B2:1648:C:O2'   | 2.27                     | 0.41              |
| 61:B2:1398:U:N3    | 61:B2:1401:U:OP2   | 2.49                     | 0.41              |
| 62:A5:56:A:O5'     | 83:Cj:48:ASN:HB3   | 2.21                     | 0.41              |
| 62:A5:95:G:N3      | 62:A5:100:G:N1     | 2.68                     | 0.41              |
| 62:A5:95:G:C2      | 62:A5:100:G:C6     | 3.09                     | 0.41              |
| 62:A5:298:U:N3     | 62:A5:300:A:O5'    | 2.54                     | 0.41              |
| 62:A5:1140:G:N3    | 62:A5:1676:A:O2'   | 2.52                     | 0.41              |
| 62:A5:1146:U:O2'   | 62:A5:1646:U:O2    | 2.39                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 62:A5:1349:A:H2'   | 62:A5:1350:A:C8    | 2.52                     | 0.41              |
| 62:A5:1713:U:H5''  | 62:A5:1755:U:H1'   | 2.02                     | 0.41              |
| 62:A5:1731:G:O2'   | 66:Cg:10:ARG:O     | 2.39                     | 0.41              |
| 62:A5:1983:A:H61   | 62:A5:2089:A:N6    | 2.17                     | 0.41              |
| 62:A5:2011:A:H2'   | 62:A5:2012:G:C8    | 2.56                     | 0.41              |
| 62:A5:3155:G:H3'   | 62:A5:3156:G:H8    | 1.85                     | 0.41              |
| 62:A5:3647:A:H2'   | 62:A5:3648:A:C8    | 2.56                     | 0.41              |
| 62:A5:3894:C:H2'   | 62:A5:3895:A:H8    | 1.86                     | 0.41              |
| 62:A5:3926:C:OP1   | 75:AI:125:ARG:NE   | 2.51                     | 0.41              |
| 63:Ac:12:LYS:HB3   | 63:Ac:27:LYS:HB3   | 2.03                     | 0.41              |
| 64:AW:90:THR:HA    | 64:AW:94:LEU:HD23  | 2.03                     | 0.41              |
| 68:AK:17:LYS:HD3   | 68:AK:89:PRO:HG3   | 2.02                     | 0.41              |
| 68:AK:57:LYS:HA    | 68:AK:57:LYS:HD3   | 1.84                     | 0.41              |
| 69:AT:42:PHE:HD1   | 69:AT:85:ASN:HA    | 1.86                     | 0.41              |
| 69:AT:50:PRO:CD    | 69:AT:51:ASP:H     | 2.31                     | 0.41              |
| 70:AF:52:VAL:HG11  | 70:AF:133:LEU:HB2  | 2.03                     | 0.41              |
| 70:AF:133:LEU:HA   | 70:AF:136:LEU:HG   | 2.03                     | 0.41              |
| 71:CF:144:THR:HG22 | 71:CF:237:PHE:HB3  | 2.03                     | 0.41              |
| 71:CF:172:ILE:HG23 | 71:CF:173:THR:H    | 1.85                     | 0.41              |
| 72:AE:201:HIS:CE1  | 72:AE:207:ILE:HG12 | 2.55                     | 0.41              |
| 72:AE:252:ARG:HA   | 72:AE:255:ARG:HD2  | 2.02                     | 0.41              |
| 73:AG:70:HIS:O     | 73:AG:98:ARG:NH2   | 2.53                     | 0.41              |
| 74:AH:35:LEU:HD12  | 74:AH:38:TYR:HB2   | 2.03                     | 0.41              |
| 76:AQ:111:LYS:HD2  | 76:AQ:111:LYS:HA   | 1.89                     | 0.41              |
| 77:CO:43:LEU:O     | 77:CO:44:ASN:ND2   | 2.54                     | 0.41              |
| 77:CO:84:LYS:HA    | 77:CO:84:LYS:HD2   | 1.82                     | 0.41              |
| 78:CL:148:GLN:HE21 | 78:CL:148:GLN:HB3  | 1.72                     | 0.41              |
| 79:CV:61:PHE:HE1   | 79:CV:81:VAL:HG23  | 1.85                     | 0.41              |
| 82:v:30:U:H2'      | 82:v:31:G:C8       | 2.56                     | 0.41              |
| 1:AA:14:ASP:HA     | 1:AA:17:LYS:HD2    | 2.02                     | 0.41              |
| 3:AB:132:THR:HA    | 3:AB:179:VAL:HG22  | 2.02                     | 0.41              |
| 3:AB:171:MET:H     | 3:AB:171:MET:HG2   | 1.67                     | 0.41              |
| 4:CB:85:ILE:HB     | 4:CB:165:HIS:HB2   | 2.04                     | 0.41              |
| 6:CC:127:LEU:HD12  | 6:CC:127:LEU:HA    | 1.88                     | 0.41              |
| 6:CC:376:LYS:HA    | 6:CC:376:LYS:HD2   | 1.80                     | 0.41              |
| 8:AU:106:ILE:HD12  | 8:AU:107:ASN:HA    | 2.03                     | 0.41              |
| 14:AN:19:ARG:H     | 14:AN:19:ARG:HD3   | 1.85                     | 0.41              |
| 15:AL:101:LYS:HE2  | 15:AL:101:LYS:HB3  | 1.84                     | 0.41              |
| 27:Ca:37:GLY:C     | 27:Ca:40:HIS:H     | 2.29                     | 0.41              |
| 27:Ca:113:LEU:HD23 | 27:Ca:113:LEU:HA   | 1.80                     | 0.41              |
| 27:Ca:124:ILE:HD13 | 27:Ca:124:ILE:HA   | 1.90                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 34:CT:4:SER:HB2    | 34:CT:5:LYS:HG3    | 2.03                     | 0.41              |
| 35:CP:40:PRO:HA    | 35:CP:113:VAL:HG12 | 2.03                     | 0.41              |
| 36:CX:163:THR:HG23 | 56:CG:56:LEU:HB2   | 2.03                     | 0.41              |
| 37:CY:54:GLU:OE2   | 37:CY:68:GLY:N     | 2.33                     | 0.41              |
| 43:CD:65:LEU:HA    | 43:CD:65:LEU:HD12  | 1.84                     | 0.41              |
| 53:CJ:123:LYS:HA   | 53:CJ:123:LYS:HD2  | 1.79                     | 0.41              |
| 55:CE:95:LEU:HA    | 55:CE:95:LEU:HD12  | 1.87                     | 0.41              |
| 61:B2:115:U:H2'    | 61:B2:116:U:C6     | 2.56                     | 0.41              |
| 61:B2:316:U:H3     | 61:B2:360:G:H1     | 1.69                     | 0.41              |
| 61:B2:411:U:H4'    | 73:AG:76:LEU:HD11  | 2.02                     | 0.41              |
| 61:B2:1426:A:H2'   | 61:B2:1428:A:C8    | 2.56                     | 0.41              |
| 61:B2:1603:G:H3'   | 61:B2:1604:A:C8    | 2.55                     | 0.41              |
| 61:B2:1615:U:H2'   | 61:B2:1616:A:C8    | 2.56                     | 0.41              |
| 61:B2:1873:A:O2'   | 73:AG:31:ARG:NH2   | 2.52                     | 0.41              |
| 62:A5:378:G:O6     | 62:A5:379:A:N6     | 2.54                     | 0.41              |
| 62:A5:937:G:N2     | 62:A5:966:U:O2'    | 2.54                     | 0.41              |
| 62:A5:1008:A:N6    | 62:A5:1009:G:O6    | 2.54                     | 0.41              |
| 62:A5:1901:G:H2'   | 62:A5:1902:U:C6    | 2.56                     | 0.41              |
| 62:A5:2031:C:H2'   | 62:A5:2032:U:C6    | 2.56                     | 0.41              |
| 62:A5:2510:A:N6    | 62:A5:2566:A:N3    | 2.69                     | 0.41              |
| 62:A5:2835:G:N2    | 62:A5:2839:A:OP2   | 2.52                     | 0.41              |
| 69:AT:11:GLN:HB3   | 69:AT:15:THR:CG2   | 2.42                     | 0.41              |
| 70:AF:66:LYS:HA    | 70:AF:66:LYS:HD2   | 1.95                     | 0.41              |
| 73:AG:64:LYS:HZ3   | 73:AG:82:SER:H     | 1.68                     | 0.41              |
| 74:AH:46:ARG:H     | 74:AH:61:TYR:HB2   | 1.85                     | 0.41              |
| 79:CV:16:ILE:HD12  | 79:CV:57:VAL:H     | 1.85                     | 0.41              |
| 79:CV:87:PRO:HB3   | 79:CV:97:TYR:HB3   | 2.03                     | 0.41              |
| 80:CM:24:LEU:HD11  | 80:CM:86:TRP:CE2   | 2.56                     | 0.41              |
| 80:CM:110:PHE:O    | 80:CM:114:TYR:N    | 2.36                     | 0.41              |
| 1:AA:14:ASP:OD1    | 1:AA:17:LYS:NZ     | 2.54                     | 0.40              |
| 1:AA:166:LYS:HD2   | 1:AA:166:LYS:HA    | 1.91                     | 0.40              |
| 6:CC:27:LEU:HD12   | 6:CC:27:LEU:HA     | 1.93                     | 0.40              |
| 6:CC:70:TRP:HE1    | 6:CC:74:ARG:NE     | 2.18                     | 0.40              |
| 6:CC:208:ARG:NH1   | 6:CC:231:GLU:OE1   | 2.53                     | 0.40              |
| 7:Ag:11:LEU:HD12   | 7:Ag:43:TRP:HZ3    | 1.85                     | 0.40              |
| 7:Ag:248:TRP:HA    | 7:Ag:261:ASP:HA    | 2.03                     | 0.40              |
| 8:AU:34:LEU:O      | 8:AU:89:ARG:NH1    | 2.54                     | 0.40              |
| 11:AM:58:ILE:HG23  | 11:AM:86:VAL:HG22  | 2.03                     | 0.40              |
| 15:AL:27:LYS:HG3   | 15:AL:29:LYS:H     | 1.86                     | 0.40              |
| 26:AJ:143:VAL:HG22 | 26:AJ:145:ILE:H    | 1.86                     | 0.40              |
| 27:Ca:8:LYS:HB2    | 62:A5:994:U:H5''   | 2.03                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 27:Ca:130:PHE:CG   | 78:CL:179:PHE:HB2  | 2.56                     | 0.40              |
| 30:CD:277:GLN:H    | 30:CD:277:GLN:HG2  | 1.67                     | 0.40              |
| 32:CR:152:SER:O    | 32:CR:156:ALA:N    | 2.53                     | 0.40              |
| 35:CP:26:PHE:CD2   | 62:A5:1688:A:H2'   | 2.56                     | 0.40              |
| 39:Cr:99:ASN:HA    | 39:Cr:102:ILE:HG22 | 2.03                     | 0.40              |
| 40:Ch:60:VAL:HA    | 40:Ch:63:GLN:HB2   | 2.03                     | 0.40              |
| 40:Ch:79:LYS:HB3   | 40:Ch:84:ARG:HD2   | 2.03                     | 0.40              |
| 46:Ci:75:LYS:HB3   | 46:Ci:75:LYS:HE2   | 1.91                     | 0.40              |
| 54:CH:31:ARG:HH12  | 54:CH:185:VAL:HB   | 1.85                     | 0.40              |
| 59:A8:42:A:N6      | 59:A8:98:U:H3      | 2.18                     | 0.40              |
| 59:A8:45:G:H2'     | 59:A8:46:C:O4'     | 2.21                     | 0.40              |
| 61:B2:169:C:H2'    | 61:B2:170:A:H8     | 1.85                     | 0.40              |
| 61:B2:1727:U:C2    | 70:AF:190:ILE:HB   | 2.55                     | 0.40              |
| 62:A5:344:U:P      | 78:CL:33:ARG:HH21  | 2.41                     | 0.40              |
| 62:A5:572:A:OP1    | 80:CM:74:ARG:NH1   | 2.54                     | 0.40              |
| 62:A5:678:U:O4     | 62:A5:742:A:N6     | 2.54                     | 0.40              |
| 62:A5:1314:U:H5'   | 71:CF:210:ASN:HD22 | 1.86                     | 0.40              |
| 62:A5:1733:A:H61   | 62:A5:2155:A:H61   | 1.68                     | 0.40              |
| 62:A5:1972:C:O2    | 62:A5:2103:G:N2    | 2.54                     | 0.40              |
| 62:A5:2282:U:OP1   | 62:A5:2461:A:O2'   | 2.39                     | 0.40              |
| 62:A5:2516:U:C2    | 62:A5:2520:U:H5    | 2.39                     | 0.40              |
| 62:A5:2792:G:H21   | 62:A5:3341:C:H5    | 1.67                     | 0.40              |
| 62:A5:3303:G:OP1   | 62:A5:3304:U:N3    | 2.54                     | 0.40              |
| 62:A5:3814:U:H2'   | 62:A5:3815:G:C8    | 2.56                     | 0.40              |
| 68:AK:16:PHE:HZ    | 68:AK:87:ILE:HG12  | 1.86                     | 0.40              |
| 69:AT:31:PRO:HD2   | 69:AT:31:PRO:O     | 2.20                     | 0.40              |
| 71:CF:112:LEU:HD23 | 71:CF:112:LEU:HA   | 1.88                     | 0.40              |
| 76:AQ:49:LEU:O     | 76:AQ:87:ARG:NH2   | 2.53                     | 0.40              |
| 78:CL:125:LEU:HA   | 78:CL:125:LEU:HD13 | 1.85                     | 0.40              |
| 78:CL:197:LYS:HD2  | 78:CL:200:LYS:HE2  | 2.02                     | 0.40              |
| 1:AA:36:GLN:O      | 1:AA:53:LYS:NZ     | 2.43                     | 0.40              |
| 1:AA:105:PRO:HA    | 1:AA:106:GLY:HA2   | 1.85                     | 0.40              |
| 5:AC:260:THR:OG1   | 5:AC:262:ARG:NH2   | 2.47                     | 0.40              |
| 6:CC:124:ARG:HH21  | 62:A5:845:C:P      | 2.44                     | 0.40              |
| 6:CC:319:LEU:HD23  | 6:CC:319:LEU:HA    | 1.80                     | 0.40              |
| 6:CC:381:ARG:NE    | 62:A5:686:U:O2'    | 2.54                     | 0.40              |
| 6:CC:383:LYS:HD3   | 6:CC:383:LYS:HA    | 1.91                     | 0.40              |
| 7:Ag:121:ILE:HB    | 7:Ag:133:TRP:CD1   | 2.56                     | 0.40              |
| 10:AX:53:GLU:O     | 10:AX:71:ARG:N     | 2.50                     | 0.40              |
| 12:AS:23:LYS:HE3   | 20:AZ:47:VAL:HG13  | 2.03                     | 0.40              |
| 26:AJ:42:ARG:HA    | 26:AJ:45:TRP:HD1   | 1.85                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 26:AJ:66:GLU:HA    | 26:AJ:67:LYS:HA    | 1.77                     | 0.40              |
| 27:Ca:40:HIS:NE2   | 62:A5:3333:A:OP2   | 2.35                     | 0.40              |
| 28:CN:11:TYR:CZ    | 28:CN:44:ARG:HG2   | 2.56                     | 0.40              |
| 28:CN:160:GLU:N    | 28:CN:160:GLU:OE2  | 2.54                     | 0.40              |
| 31:CQ:11:ARG:HH11  | 31:CQ:13:VAL:HA    | 1.86                     | 0.40              |
| 31:CQ:163:THR:O    | 31:CQ:163:THR:OG1  | 2.27                     | 0.40              |
| 31:CQ:180:ARG:HH21 | 31:CQ:188:LYS:HZ1  | 1.69                     | 0.40              |
| 32:CR:110:ARG:HA   | 32:CR:120:TYR:OH   | 2.21                     | 0.40              |
| 44:Ce:42:ASN:O     | 44:Ce:46:ARG:NE    | 2.52                     | 0.40              |
| 46:Ci:44:THR:HG23  | 46:Ci:47:THR:H     | 1.86                     | 0.40              |
| 46:Ci:65:LYS:HB3   | 46:Ci:65:LYS:HE2   | 1.86                     | 0.40              |
| 46:Ci:87:LEU:HD23  | 46:Ci:87:LEU:HA    | 1.81                     | 0.40              |
| 49:Cm:97:ARG:HE    | 49:Cm:122:ARG:NE   | 2.19                     | 0.40              |
| 54:CH:34:LEU:HD23  | 54:CH:78:MET:HE3   | 2.03                     | 0.40              |
| 58:A7:15:C:H2'     | 58:A7:16:A:C8      | 2.56                     | 0.40              |
| 59:A8:10:C:H2'     | 59:A8:11:G:C8      | 2.56                     | 0.40              |
| 60:Cz:203:SER:HB3  | 60:Cz:215:ARG:HH21 | 1.86                     | 0.40              |
| 61:B2:332:U:H2'    | 61:B2:333:A:H8     | 1.85                     | 0.40              |
| 61:B2:420:U:O2'    | 61:B2:423:G:O6     | 2.36                     | 0.40              |
| 61:B2:912:U:H2'    | 61:B2:913:G:H4'    | 2.03                     | 0.40              |
| 62:A5:295:G:H2'    | 62:A5:296:C:C6     | 2.56                     | 0.40              |
| 62:A5:517:A:H2'    | 62:A5:518:G:C8     | 2.56                     | 0.40              |
| 62:A5:670:G:O6     | 62:A5:1562:U:O2'   | 2.28                     | 0.40              |
| 62:A5:764:A:H3'    | 62:A5:765:A:C8     | 2.56                     | 0.40              |
| 62:A5:794:G:H2'    | 62:A5:2750:A:C6    | 2.56                     | 0.40              |
| 62:A5:872:A:O5'    | 62:A5:983:U:O2'    | 2.26                     | 0.40              |
| 62:A5:1712:C:H2'   | 62:A5:1713:U:H5'   | 2.03                     | 0.40              |
| 62:A5:3226:A:H2'   | 62:A5:3227:A:C8    | 2.56                     | 0.40              |
| 62:A5:3444:G:O6    | 62:A5:3664:A:N6    | 2.54                     | 0.40              |
| 71:CF:49:ARG:NE    | 71:CF:189:GLN:OE1  | 2.54                     | 0.40              |
| 71:CF:77:LEU:O     | 71:CF:81:ARG:N     | 2.49                     | 0.40              |
| 72:AE:63:LYS:O     | 72:AE:67:GLN:N     | 2.52                     | 0.40              |
| 74:AH:141:ARG:HG3  | 74:AH:155:HIS:HE1  | 1.86                     | 0.40              |
| 2:CA:41:ILE:HG22   | 2:CA:90:CYS:HB2    | 2.03                     | 0.40              |
| 5:AC:127:SER:HB3   | 5:AC:133:ALA:HB2   | 2.02                     | 0.40              |
| 6:CC:274:SER:OG    | 6:CC:275:THR:N     | 2.54                     | 0.40              |
| 7:Ag:158:SER:HA    | 7:Ag:201:VAL:HG21  | 2.03                     | 0.40              |
| 11:AM:39:VAL:H     | 11:AM:40:HIS:HA    | 1.86                     | 0.40              |
| 12:AS:28:ILE:HG13  | 61:B2:1731:U:C4    | 2.56                     | 0.40              |
| 17:AP:47:ARG:NH2   | 61:B2:1747:A:O2'   | 2.35                     | 0.40              |
| 18:AV:15:ARG:NH1   | 18:AV:33:GLN:OE1   | 2.53                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 18:AV:51:LYS:HE2   | 18:AV:51:LYS:HB2   | 1.94                     | 0.40              |
| 19:AY:16:ASN:HB2   | 19:AY:23:GLN:HG2   | 2.03                     | 0.40              |
| 20:AZ:75:ARG:HA    | 20:AZ:75:ARG:HD3   | 1.72                     | 0.40              |
| 23:AD:70:GLU:HG2   | 23:AD:74:MET:HE3   | 2.03                     | 0.40              |
| 26:AJ:94:LYS:NZ    | 26:AJ:96:ASP:HB3   | 2.36                     | 0.40              |
| 28:CN:35:LYS:NZ    | 62:A5:1787:C:OP2   | 2.35                     | 0.40              |
| 28:CN:106:VAL:HG21 | 28:CN:132:VAL:HG21 | 2.02                     | 0.40              |
| 30:CD:200:PHE:HB3  | 30:CD:237:GLU:HB3  | 2.02                     | 0.40              |
| 31:CQ:7:HIS:HB3    | 31:CQ:8:LYS:H      | 1.60                     | 0.40              |
| 31:CQ:18:PRO:HD2   | 31:CQ:26:ARG:NH1   | 2.37                     | 0.40              |
| 32:CR:100:ARG:HD3  | 62:A5:2035:C:OP1   | 2.21                     | 0.40              |
| 35:CP:59:PRO:HG3   | 35:CP:76:TRP:CD2   | 2.57                     | 0.40              |
| 37:CY:50:ARG:NH1   | 37:CY:109:LEU:HB3  | 2.36                     | 0.40              |
| 39:Cr:16:ASN:CG    | 39:Cr:18:PHE:H     | 2.29                     | 0.40              |
| 45:Cf:139:LEU:HD23 | 45:Cf:139:LEU:HA   | 1.70                     | 0.40              |
| 53:CJ:96:GLU:O     | 53:CJ:98:GLU:N     | 2.54                     | 0.40              |
| 55:CE:142:GLN:H    | 55:CE:142:GLN:HG3  | 1.65                     | 0.40              |
| 55:CE:220:LYS:HG3  | 80:CM:110:PHE:H    | 1.85                     | 0.40              |
| 58:A7:17:C:H2'     | 58:A7:18:G:H8      | 1.87                     | 0.40              |
| 59:A8:111:G:OP1    | 62:A5:2147:C:O2'   | 2.37                     | 0.40              |
| 60:Cz:21:SER:OG    | 60:Cz:174:MET:O    | 2.29                     | 0.40              |
| 61:B2:358:A:N6     | 61:B2:359:C:N3     | 2.69                     | 0.40              |
| 61:B2:1549:U:H1'   | 61:B2:1567:A:C6    | 2.56                     | 0.40              |
| 62:A5:505:U:H2'    | 62:A5:506:A:C8     | 2.56                     | 0.40              |
| 62:A5:1209:A:H3'   | 62:A5:1210:A:H8    | 1.86                     | 0.40              |
| 62:A5:1226:G:H21   | 62:A5:1227:C:H41   | 1.69                     | 0.40              |
| 62:A5:1350:A:H1'   | 62:A5:3168:A:N1    | 2.37                     | 0.40              |
| 62:A5:1577:A:N6    | 62:A5:1578:C:O2    | 2.54                     | 0.40              |
| 62:A5:3578:A:OP1   | 79:CV:51:ARG:NH2   | 2.55                     | 0.40              |
| 62:A5:3678:G:N2    | 62:A5:3679:C:O2    | 2.55                     | 0.40              |
| 63:Ac:43:LYS:HE3   | 70:AF:165:VAL:HG22 | 2.03                     | 0.40              |
| 69:AT:122:LYS:HZ2  | 69:AT:128:GLN:HE22 | 1.68                     | 0.40              |
| 71:CF:127:LYS:HB3  | 71:CF:127:LYS:HE2  | 1.90                     | 0.40              |
| 71:CF:224:TRP:CH2  | 71:CF:247:LEU:HD21 | 2.57                     | 0.40              |
| 74:AH:20:LYS:HE3   | 74:AH:20:LYS:HB3   | 1.91                     | 0.40              |
| 76:AQ:50:GLN:HA    | 76:AQ:53:LEU:HD12  | 2.03                     | 0.40              |
| 77:CO:41:GLU:OE2   | 77:CO:41:GLU:N     | 2.53                     | 0.40              |
| 78:CL:130:GLU:O    | 78:CL:132:LYS:NZ   | 2.45                     | 0.40              |
| 83:Cj:33:LYS:HE2   | 83:Cj:33:LYS:HB2   | 1.82                     | 0.40              |
| 83:Cj:54:LYS:C     | 83:Cj:56:ARG:N     | 2.80                     | 0.40              |
| 1:AA:32:PHE:CD2    | 61:B2:1127:G:H5'   | 2.57                     | 0.40              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 2:CA:19:HIS:CE1    | 2:CA:194:ASN:HB2  | 2.56                     | 0.40              |
| 4:CB:16:PHE:HB2    | 4:CB:17:TYR:CE2   | 2.57                     | 0.40              |
| 4:CB:393:LYS:HB3   | 62:A5:3944:A:H5'  | 2.03                     | 0.40              |
| 5:AC:111:VAL:HG11  | 5:AC:138:ILE:HG22 | 2.04                     | 0.40              |
| 6:CC:3:LEU:HD21    | 62:A5:503:A:H2    | 1.87                     | 0.40              |
| 6:CC:237:LYS:HE3   | 62:A5:843:A:H2    | 1.86                     | 0.40              |
| 11:AM:112:GLY:O    | 61:B2:1314:G:O2'  | 2.40                     | 0.40              |
| 14:AN:3:ARG:NH2    | 61:B2:953:A:OP2   | 2.39                     | 0.40              |
| 15:AL:105:ASN:OD1  | 61:B2:354:U:OP1   | 2.39                     | 0.40              |
| 16:AR:6:THR:OG1    | 16:AR:7:LYS:N     | 2.52                     | 0.40              |
| 17:AP:32:PRO:HB3   | 17:AP:35:GLN:HG2  | 2.04                     | 0.40              |
| 21:Aa:92:ARG:HB3   | 61:B2:1991:C:C6   | 2.57                     | 0.40              |
| 26:AJ:146:PRO:HD2  | 61:B2:479:A:H5''  | 2.02                     | 0.40              |
| 30:CD:35:ARG:NH1   | 62:A5:3193:C:OP1  | 2.54                     | 0.40              |
| 30:CD:38:PHE:C     | 30:CD:48:LYS:HZ1  | 2.29                     | 0.40              |
| 30:CD:267:ARG:NE   | 30:CD:270:ALA:H   | 2.19                     | 0.40              |
| 31:CQ:45:ARG:HD2   | 31:CQ:45:ARG:HA   | 1.91                     | 0.40              |
| 33:CS:111:ARG:NH2  | 62:A5:1538:U:O2'  | 2.55                     | 0.40              |
| 38:CZ:3:LYS:HD3    | 38:CZ:3:LYS:HA    | 1.94                     | 0.40              |
| 44:Ce:7:TYR:HD1    | 44:Ce:7:TYR:HA    | 1.74                     | 0.40              |
| 54:CH:43:LEU:HD23  | 54:CH:43:LEU:HA   | 1.89                     | 0.40              |
| 54:CH:84:PHE:HD1   | 54:CH:186:VAL:HB  | 1.86                     | 0.40              |
| 54:CH:115:PHE:HA   | 54:CH:116:LEU:HA  | 1.77                     | 0.40              |
| 55:CE:143:ARG:HD3  | 55:CE:143:ARG:HA  | 1.80                     | 0.40              |
| 59:A8:34:C:OP1     | 83:Cj:70:LEU:HD13 | 2.08                     | 0.40              |
| 59:A8:111:G:H8     | 59:A8:111:G:P     | 2.44                     | 0.40              |
| 60:Cz:194:LEU:HD23 | 60:Cz:194:LEU:HA  | 1.90                     | 0.40              |
| 61:B2:76:A:N1      | 73:AG:154:ARG:NH1 | 2.70                     | 0.40              |
| 61:B2:259:G:H2'    | 61:B2:260:A:H8    | 1.86                     | 0.40              |
| 61:B2:334:G:H2'    | 61:B2:335:U:H6    | 1.86                     | 0.40              |
| 61:B2:713:A:N6     | 74:AH:108:ASN:O   | 2.54                     | 0.40              |
| 61:B2:909:U:H2'    | 61:B2:934:A:N1    | 2.37                     | 0.40              |
| 61:B2:1444:C:C3'   | 69:AT:129:ARG:CZ  | 2.99                     | 0.40              |
| 61:B2:1729:C:H42   | 61:B2:1763:C:H3'  | 1.87                     | 0.40              |
| 61:B2:1783:U:H5'   | 69:AT:92:PHE:CD2  | 2.57                     | 0.40              |
| 62:A5:483:U:H2'    | 62:A5:484:A:H8    | 1.86                     | 0.40              |
| 62:A5:613:U:H2'    | 62:A5:614:G:C8    | 2.56                     | 0.40              |
| 62:A5:653:U:H2'    | 62:A5:654:G:C8    | 2.55                     | 0.40              |
| 62:A5:669:U:N3     | 62:A5:1594:U:O4   | 2.55                     | 0.40              |
| 62:A5:1006:A:C6    | 62:A5:1136:A:H2   | 2.39                     | 0.40              |
| 62:A5:1391:A:N6    | 62:A5:1392:A:N1   | 2.70                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 62:A5:2111:A:C6    | 62:A5:2112:A:C6    | 3.10                     | 0.40              |
| 62:A5:2115:U:H2'   | 62:A5:2116:U:C6    | 2.57                     | 0.40              |
| 62:A5:2247:U:H6    | 62:A5:2247:U:H2'   | 1.74                     | 0.40              |
| 62:A5:2633:A:OP2   | 62:A5:2639:G:N2    | 2.47                     | 0.40              |
| 62:A5:3339:U:N3    | 62:A5:3342:C:N3    | 2.69                     | 0.40              |
| 62:A5:3820:C:H42   | 80:CM:147:ARG:HD2  | 1.86                     | 0.40              |
| 71:CF:46:ILE:O     | 71:CF:50:LYS:N     | 2.52                     | 0.40              |
| 73:AG:142:ARG:HG3  | 73:AG:148:SER:HA   | 2.03                     | 0.40              |
| 74:AH:102:PRO:HG2  | 74:AH:107:ARG:HB3  | 2.03                     | 0.40              |
| 77:CO:129:LEU:HD23 | 77:CO:129:LEU:HA   | 1.91                     | 0.40              |
| 79:CV:109:LYS:HD2  | 79:CV:109:LYS:HA   | 1.66                     | 0.40              |
| 2:CA:188:LYS:HA    | 2:CA:188:LYS:HD2   | 1.89                     | 0.40              |
| 4:CB:87:VAL:HG21   | 4:CB:110:LEU:HD23  | 2.03                     | 0.40              |
| 5:AC:81:LEU:HB3    | 5:AC:82:GLY:H      | 1.81                     | 0.40              |
| 6:CC:176:ARG:NE    | 62:A5:225:U:OP1    | 2.44                     | 0.40              |
| 9:AO:46:ASP:HB3    | 9:AO:49:GLY:H      | 1.87                     | 0.40              |
| 9:AO:143:LYS:NZ    | 61:B2:1096:C:OP1   | 2.34                     | 0.40              |
| 10:AX:90:SER:HB2   | 10:AX:134:TYR:HE1  | 1.86                     | 0.40              |
| 10:AX:128:VAL:HG11 | 10:AX:141:PRO:HG3  | 2.04                     | 0.40              |
| 11:AM:56:LEU:HD12  | 11:AM:136:ARG:HH22 | 1.87                     | 0.40              |
| 11:AM:131:VAL:HG22 | 11:AM:135:LEU:HD23 | 2.04                     | 0.40              |
| 16:AR:115:ARG:H    | 16:AR:115:ARG:HG2  | 1.62                     | 0.40              |
| 26:AJ:76:ASN:HD21  | 72:AE:252:ARG:NH2  | 2.19                     | 0.40              |
| 26:AJ:113:THR:HA   | 26:AJ:116:PHE:HB3  | 2.03                     | 0.40              |
| 26:AJ:163:LYS:HE3  | 26:AJ:163:LYS:HB3  | 1.95                     | 0.40              |
| 28:CN:12:ARG:NH1   | 62:A5:286:A:N7     | 2.70                     | 0.40              |
| 28:CN:75:VAL:HA    | 28:CN:76:PRO:HD3   | 1.88                     | 0.40              |
| 30:CD:140:GLY:N    | 62:A5:1293:A:O4'   | 2.54                     | 0.40              |
| 30:CD:155:THR:HG23 | 30:CD:179:ARG:HA   | 2.02                     | 0.40              |
| 31:CQ:65:ARG:HD3   | 62:A5:872:A:N7     | 2.35                     | 0.40              |
| 36:CX:178:SER:OG   | 36:CX:178:SER:O    | 2.33                     | 0.40              |
| 43:Cd:37:LYS:HD2   | 43:Cd:37:LYS:HA    | 1.66                     | 0.40              |
| 50:Cn:11:ARG:HD3   | 61:B2:1214:A:H5'   | 2.04                     | 0.40              |
| 54:CH:12:ILE:HD13  | 54:CH:12:ILE:HA    | 1.92                     | 0.40              |
| 61:B2:215:C:O2'    | 61:B2:916:U:OP1    | 2.35                     | 0.40              |
| 61:B2:489:C:H41    | 61:B2:507:C:H42    | 1.68                     | 0.40              |
| 61:B2:896:A:N7     | 74:AH:113:LYS:HB2  | 2.37                     | 0.40              |
| 61:B2:1452:U:H2'   | 61:B2:1453:G:C8    | 2.57                     | 0.40              |
| 61:B2:1697:A:C5    | 61:B2:1698:G:H1'   | 2.56                     | 0.40              |
| 62:A5:362:A:O2'    | 62:A5:1670:G:O6    | 2.37                     | 0.40              |
| 62:A5:1019:U:H2'   | 62:A5:1020:A:C8    | 2.56                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 62:A5:1100:G:H2'  | 62:A5:1101:A:H8   | 1.87                     | 0.40              |
| 62:A5:1105:U:O2'  | 62:A5:1110:G:O3'  | 2.29                     | 0.40              |
| 62:A5:1525:G:H2'  | 62:A5:1526:G:C8   | 2.57                     | 0.40              |
| 62:A5:2051:A:H2'  | 62:A5:2052:G:C8   | 2.57                     | 0.40              |
| 62:A5:2123:G:H2'  | 62:A5:2124:G:H8   | 1.87                     | 0.40              |
| 62:A5:2600:A:N6   | 62:A5:2601:A:N1   | 2.69                     | 0.40              |
| 77:CO:51:ARG:O    | 77:CO:54:ILE:N    | 2.48                     | 0.40              |
| 79:CV:40:ILE:HG21 | 79:CV:40:ILE:HD13 | 1.90                     | 0.40              |
| 79:CV:131:ARG:HD3 | 79:CV:131:ARG:HA  | 1.95                     | 0.40              |
| 80:CM:110:PHE:HD1 | 80:CM:110:PHE:HA  | 1.73                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed       | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|----------------|-----------|----------|----------|-------------|-----|
| 1   | AA    | 216/218 (99%)  | 188 (87%) | 27 (12%) | 1 (0%)   | 24          | 63  |
| 2   | CA    | 251/253 (99%)  | 197 (78%) | 52 (21%) | 2 (1%)   | 16          | 52  |
| 3   | AB    | 218/220 (99%)  | 186 (85%) | 29 (13%) | 3 (1%)   | 9           | 39  |
| 4   | CB    | 412/414 (100%) | 327 (79%) | 84 (20%) | 1 (0%)   | 43          | 77  |
| 5   | AC    | 225/227 (99%)  | 200 (89%) | 25 (11%) | 0        | 100         | 100 |
| 6   | CC    | 390/392 (100%) | 308 (79%) | 82 (21%) | 0        | 100         | 100 |
| 7   | Ag    | 316/318 (99%)  | 276 (87%) | 40 (13%) | 0        | 100         | 100 |
| 8   | AU    | 100/102 (98%)  | 93 (93%)  | 7 (7%)   | 0        | 100         | 100 |
| 9   | AO    | 132/134 (98%)  | 112 (85%) | 19 (14%) | 1 (1%)   | 16          | 52  |
| 10  | AX    | 141/143 (99%)  | 112 (79%) | 29 (21%) | 0        | 100         | 100 |
| 11  | AM    | 117/119 (98%)  | 100 (86%) | 17 (14%) | 0        | 100         | 100 |
| 12  | AS    | 135/137 (98%)  | 120 (89%) | 15 (11%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 13  | Ad    | 50/52 (96%)   | 38 (76%)  | 12 (24%) | 0        | 100         | 100 |
| 14  | AN    | 148/150 (99%) | 137 (93%) | 11 (7%)  | 0        | 100         | 100 |
| 15  | AL    | 153/155 (99%) | 127 (83%) | 26 (17%) | 0        | 100         | 100 |
| 16  | AR    | 118/120 (98%) | 107 (91%) | 11 (9%)  | 0        | 100         | 100 |
| 17  | AP    | 122/124 (98%) | 108 (88%) | 14 (12%) | 0        | 100         | 100 |
| 18  | AV    | 80/82 (98%)   | 67 (84%)  | 13 (16%) | 0        | 100         | 100 |
| 19  | AY    | 124/126 (98%) | 106 (86%) | 18 (14%) | 0        | 100         | 100 |
| 20  | AZ    | 72/74 (97%)   | 59 (82%)  | 13 (18%) | 0        | 100         | 100 |
| 21  | Aa    | 105/107 (98%) | 85 (81%)  | 20 (19%) | 0        | 100         | 100 |
| 22  | Ab    | 82/84 (98%)   | 66 (80%)  | 16 (20%) | 0        | 100         | 100 |
| 23  | AD    | 225/227 (99%) | 191 (85%) | 33 (15%) | 1 (0%)   | 30          | 67  |
| 24  | Ae    | 56/58 (97%)   | 39 (70%)  | 17 (30%) | 0        | 100         | 100 |
| 25  | Af    | 78/80 (98%)   | 64 (82%)  | 14 (18%) | 0        | 100         | 100 |
| 26  | AJ    | 179/181 (99%) | 156 (87%) | 22 (12%) | 1 (1%)   | 21          | 58  |
| 27  | Ca    | 147/149 (99%) | 112 (76%) | 34 (23%) | 1 (1%)   | 18          | 55  |
| 28  | CN    | 201/203 (99%) | 153 (76%) | 46 (23%) | 2 (1%)   | 12          | 47  |
| 29  | CI    | 215/217 (99%) | 184 (86%) | 31 (14%) | 0        | 100         | 100 |
| 30  | CD    | 288/290 (99%) | 247 (86%) | 40 (14%) | 1 (0%)   | 36          | 71  |
| 31  | CQ    | 185/187 (99%) | 152 (82%) | 32 (17%) | 1 (0%)   | 24          | 63  |
| 32  | CR    | 201/203 (99%) | 182 (90%) | 19 (10%) | 0        | 100         | 100 |
| 33  | CS    | 171/173 (99%) | 127 (74%) | 41 (24%) | 3 (2%)   | 6           | 33  |
| 34  | CT    | 156/158 (99%) | 118 (76%) | 37 (24%) | 1 (1%)   | 21          | 58  |
| 35  | CP    | 183/185 (99%) | 153 (84%) | 30 (16%) | 0        | 100         | 100 |
| 36  | CX    | 118/120 (98%) | 94 (80%)  | 23 (20%) | 1 (1%)   | 16          | 52  |
| 37  | CY    | 129/131 (98%) | 111 (86%) | 18 (14%) | 0        | 100         | 100 |
| 38  | CZ    | 132/134 (98%) | 112 (85%) | 20 (15%) | 0        | 100         | 100 |
| 39  | Cr    | 132/134 (98%) | 92 (70%)  | 37 (28%) | 3 (2%)   | 5           | 28  |
| 40  | Ch    | 121/123 (98%) | 107 (88%) | 14 (12%) | 0        | 100         | 100 |
| 41  | Cb    | 73/75 (97%)   | 56 (77%)  | 17 (23%) | 0        | 100         | 100 |
| 42  | Cc    | 98/100 (98%)  | 94 (96%)  | 4 (4%)   | 0        | 100         | 100 |
| 43  | Cd    | 109/111 (98%) | 89 (82%)  | 20 (18%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 44  | Ce    | 130/132 (98%) | 99 (76%)  | 31 (24%) | 0        | 100         | 100 |
| 45  | Cf    | 155/157 (99%) | 119 (77%) | 34 (22%) | 2 (1%)   | 9           | 41  |
| 46  | Ci    | 111/113 (98%) | 82 (74%)  | 29 (26%) | 0        | 100         | 100 |
| 47  | Ck    | 68/70 (97%)   | 63 (93%)  | 5 (7%)   | 0        | 100         | 100 |
| 48  | Cl    | 48/50 (96%)   | 33 (69%)  | 14 (29%) | 1 (2%)   | 5           | 29  |
| 49  | Cm    | 50/52 (96%)   | 41 (82%)  | 9 (18%)  | 0        | 100         | 100 |
| 50  | Cn    | 23/25 (92%)   | 21 (91%)  | 2 (9%)   | 0        | 100         | 100 |
| 51  | Cp    | 89/91 (98%)   | 72 (81%)  | 17 (19%) | 0        | 100         | 100 |
| 52  | Co    | 102/104 (98%) | 79 (78%)  | 23 (22%) | 0        | 100         | 100 |
| 53  | CJ    | 180/182 (99%) | 147 (82%) | 32 (18%) | 1 (1%)   | 21          | 58  |
| 54  | CH    | 188/190 (99%) | 165 (88%) | 23 (12%) | 0        | 100         | 100 |
| 55  | CE    | 226/228 (99%) | 178 (79%) | 46 (20%) | 2 (1%)   | 14          | 49  |
| 56  | CG    | 239/241 (99%) | 205 (86%) | 31 (13%) | 3 (1%)   | 9           | 41  |
| 60  | Cz    | 215/217 (99%) | 192 (89%) | 23 (11%) | 0        | 100         | 100 |
| 63  | Ac    | 60/62 (97%)   | 53 (88%)  | 7 (12%)  | 0        | 100         | 100 |
| 64  | AW    | 127/129 (98%) | 109 (86%) | 18 (14%) | 0        | 100         | 100 |
| 65  | CW    | 56/58 (97%)   | 45 (80%)  | 11 (20%) | 0        | 100         | 100 |
| 66  | Cg    | 102/104 (98%) | 88 (86%)  | 14 (14%) | 0        | 100         | 100 |
| 67  | CU    | 94/96 (98%)   | 76 (81%)  | 18 (19%) | 0        | 100         | 100 |
| 68  | AK    | 88/90 (98%)   | 68 (77%)  | 19 (22%) | 1 (1%)   | 11          | 45  |
| 69  | AT    | 128/143 (90%) | 104 (81%) | 20 (16%) | 4 (3%)   | 3           | 21  |
| 70  | AF    | 187/189 (99%) | 158 (84%) | 28 (15%) | 1 (0%)   | 24          | 63  |
| 71  | CF    | 224/226 (99%) | 188 (84%) | 32 (14%) | 4 (2%)   | 6           | 33  |
| 72  | AE    | 259/261 (99%) | 225 (87%) | 34 (13%) | 0        | 100         | 100 |
| 73  | AG    | 229/231 (99%) | 211 (92%) | 18 (8%)  | 0        | 100         | 100 |
| 74  | AH    | 192/194 (99%) | 161 (84%) | 31 (16%) | 0        | 100         | 100 |
| 75  | AI    | 205/207 (99%) | 162 (79%) | 40 (20%) | 3 (2%)   | 8           | 38  |
| 76  | AQ    | 146/148 (99%) | 117 (80%) | 28 (19%) | 1 (1%)   | 18          | 55  |
| 77  | CO    | 203/205 (99%) | 161 (79%) | 38 (19%) | 4 (2%)   | 6           | 31  |
| 78  | CL    | 208/210 (99%) | 151 (73%) | 54 (26%) | 3 (1%)   | 9           | 39  |
| 79  | CV    | 132/134 (98%) | 115 (87%) | 17 (13%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed          | Favoured   | Allowed    | Outliers | Percentiles |     |
|-----|-------|-------------------|------------|------------|----------|-------------|-----|
| 80  | CM    | 157/159 (99%)     | 131 (83%)  | 26 (17%)   | 0        | 100         | 100 |
| 83  | Cj    | 85/87 (98%)       | 57 (67%)   | 25 (29%)   | 3 (4%)   | 3           | 20  |
| All | All   | 11610/11775 (99%) | 9628 (83%) | 1926 (17%) | 56 (0%)  | 26          | 63  |

All (56) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | AB    | 120 | TRP  |
| 69  | AT    | 40  | ALA  |
| 71  | CF    | 237 | PHE  |
| 77  | CO    | 113 | PRO  |
| 30  | CD    | 20  | PHE  |
| 48  | Cl    | 50  | LYS  |
| 56  | CG    | 44  | PHE  |
| 71  | CF    | 171 | PRO  |
| 71  | CF    | 173 | THR  |
| 75  | AI    | 99  | ASN  |
| 1   | AA    | 32  | PHE  |
| 27  | Ca    | 79  | LEU  |
| 28  | CN    | 125 | ALA  |
| 33  | CS    | 119 | ALA  |
| 39  | Cr    | 28  | PRO  |
| 78  | CL    | 53  | ALA  |
| 83  | Cj    | 29  | LEU  |
| 83  | Cj    | 45  | ARG  |
| 3   | AB    | 184 | LEU  |
| 23  | AD    | 202 | PRO  |
| 33  | CS    | 173 | ARG  |
| 39  | Cr    | 27  | LYS  |
| 39  | Cr    | 73  | TYR  |
| 56  | CG    | 168 | PRO  |
| 68  | AK    | 61  | ALA  |
| 75  | AI    | 21  | LEU  |
| 2   | CA    | 143 | THR  |
| 3   | AB    | 119 | LYS  |
| 45  | Cf    | 139 | LEU  |
| 53  | CJ    | 97  | TYR  |
| 55  | CE    | 61  | PRO  |
| 69  | AT    | 50  | PRO  |
| 77  | CO    | 112 | SER  |
| 78  | CL    | 61  | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 78  | CL    | 125 | LEU  |
| 9   | AO    | 141 | ARG  |
| 26  | AJ    | 7   | PRO  |
| 31  | CQ    | 3   | ILE  |
| 69  | AT    | 89  | PRO  |
| 75  | AI    | 143 | ARG  |
| 83  | Cj    | 55  | GLY  |
| 55  | CE    | 60  | VAL  |
| 56  | CG    | 109 | PRO  |
| 28  | CN    | 45  | PRO  |
| 69  | AT    | 49  | ASP  |
| 70  | AF    | 129 | GLY  |
| 2   | CA    | 210 | PRO  |
| 36  | CX    | 165 | VAL  |
| 45  | Cf    | 108 | PRO  |
| 76  | AQ    | 61  | GLY  |
| 77  | CO    | 111 | PRO  |
| 77  | CO    | 202 | GLY  |
| 4   | CB    | 40  | PRO  |
| 33  | CS    | 133 | PRO  |
| 34  | CT    | 147 | PRO  |
| 71  | CF    | 106 | PRO  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 1   | AA    | 190/190 (100%) | 189 (100%) | 1 (0%)   | 81          | 82  |
| 2   | CA    | 195/195 (100%) | 190 (97%)  | 5 (3%)   | 40          | 61  |
| 3   | AB    | 199/199 (100%) | 198 (100%) | 1 (0%)   | 81          | 82  |
| 4   | CB    | 349/349 (100%) | 342 (98%)  | 7 (2%)   | 48          | 66  |
| 5   | AC    | 188/188 (100%) | 188 (100%) | 0        | 100         | 100 |
| 6   | CC    | 323/323 (100%) | 315 (98%)  | 8 (2%)   | 42          | 62  |
| 7   | Ag    | 280/280 (100%) | 277 (99%)  | 3 (1%)   | 65          | 74  |

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 8   | AU    | 95/95 (100%)   | 95 (100%)  | 0        | 100         | 100 |
| 9   | AO    | 103/103 (100%) | 101 (98%)  | 2 (2%)   | 50          | 66  |
| 10  | AX    | 116/116 (100%) | 115 (99%)  | 1 (1%)   | 70          | 77  |
| 11  | AM    | 104/104 (100%) | 104 (100%) | 0        | 100         | 100 |
| 12  | AS    | 123/123 (100%) | 123 (100%) | 0        | 100         | 100 |
| 13  | Ad    | 45/45 (100%)   | 44 (98%)   | 1 (2%)   | 45          | 64  |
| 14  | AN    | 130/130 (100%) | 128 (98%)  | 2 (2%)   | 57          | 71  |
| 15  | AL    | 138/138 (100%) | 137 (99%)  | 1 (1%)   | 76          | 79  |
| 16  | AR    | 108/108 (100%) | 107 (99%)  | 1 (1%)   | 70          | 77  |
| 17  | AP    | 111/111 (100%) | 110 (99%)  | 1 (1%)   | 70          | 77  |
| 18  | AV    | 67/67 (100%)   | 67 (100%)  | 0        | 100         | 100 |
| 19  | AY    | 105/106 (99%)  | 105 (100%) | 0        | 100         | 100 |
| 20  | AZ    | 67/67 (100%)   | 66 (98%)   | 1 (2%)   | 57          | 71  |
| 21  | Aa    | 94/94 (100%)   | 93 (99%)   | 1 (1%)   | 65          | 74  |
| 22  | Ab    | 72/72 (100%)   | 71 (99%)   | 1 (1%)   | 59          | 72  |
| 23  | AD    | 192/192 (100%) | 192 (100%) | 0        | 100         | 100 |
| 24  | Ae    | 47/47 (100%)   | 47 (100%)  | 0        | 100         | 100 |
| 25  | Af    | 70/70 (100%)   | 70 (100%)  | 0        | 100         | 100 |
| 26  | AJ    | 161/161 (100%) | 159 (99%)  | 2 (1%)   | 63          | 74  |
| 27  | Ca    | 122/122 (100%) | 120 (98%)  | 2 (2%)   | 55          | 69  |
| 28  | CN    | 174/174 (100%) | 172 (99%)  | 2 (1%)   | 65          | 74  |
| 29  | CI    | 187/187 (100%) | 185 (99%)  | 2 (1%)   | 65          | 74  |
| 30  | CD    | 241/241 (100%) | 240 (100%) | 1 (0%)   | 84          | 83  |
| 31  | CQ    | 164/164 (100%) | 160 (98%)  | 4 (2%)   | 43          | 63  |
| 32  | CR    | 176/176 (100%) | 172 (98%)  | 4 (2%)   | 44          | 63  |
| 33  | CS    | 156/156 (100%) | 154 (99%)  | 2 (1%)   | 61          | 72  |
| 34  | CT    | 137/137 (100%) | 135 (98%)  | 2 (2%)   | 57          | 71  |
| 35  | CP    | 160/160 (100%) | 157 (98%)  | 3 (2%)   | 50          | 66  |
| 36  | CX    | 106/106 (100%) | 105 (99%)  | 1 (1%)   | 70          | 77  |
| 37  | CY    | 116/116 (100%) | 114 (98%)  | 2 (2%)   | 53          | 68  |
| 38  | CZ    | 121/121 (100%) | 121 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed       | Rotameric  | Outliers | Percentiles |     |
|-----|-------|----------------|------------|----------|-------------|-----|
| 39  | Cr    | 112/112 (100%) | 111 (99%)  | 1 (1%)   | 70          | 77  |
| 40  | Ch    | 112/112 (100%) | 110 (98%)  | 2 (2%)   | 51          | 67  |
| 41  | Cb    | 67/67 (100%)   | 67 (100%)  | 0        | 100         | 100 |
| 42  | Cc    | 84/84 (100%)   | 82 (98%)   | 2 (2%)   | 43          | 63  |
| 43  | Cd    | 103/103 (100%) | 101 (98%)  | 2 (2%)   | 50          | 66  |
| 44  | Ce    | 120/120 (100%) | 116 (97%)  | 4 (3%)   | 33          | 55  |
| 45  | Cf    | 123/123 (100%) | 119 (97%)  | 4 (3%)   | 33          | 55  |
| 46  | Ci    | 100/100 (100%) | 98 (98%)   | 2 (2%)   | 48          | 66  |
| 47  | Ck    | 65/65 (100%)   | 65 (100%)  | 0        | 100         | 100 |
| 48  | Cl    | 45/45 (100%)   | 45 (100%)  | 0        | 100         | 100 |
| 49  | Cm    | 48/48 (100%)   | 48 (100%)  | 0        | 100         | 100 |
| 50  | Cn    | 23/23 (100%)   | 23 (100%)  | 0        | 100         | 100 |
| 51  | Cp    | 74/74 (100%)   | 73 (99%)   | 1 (1%)   | 59          | 72  |
| 52  | Co    | 94/94 (100%)   | 94 (100%)  | 0        | 100         | 100 |
| 53  | CJ    | 155/155 (100%) | 154 (99%)  | 1 (1%)   | 78          | 81  |
| 54  | CH    | 169/169 (100%) | 168 (99%)  | 1 (1%)   | 78          | 81  |
| 55  | CE    | 197/197 (100%) | 194 (98%)  | 3 (2%)   | 57          | 71  |
| 56  | CG    | 210/210 (100%) | 209 (100%) | 1 (0%)   | 81          | 82  |
| 60  | Cz    | 190/190 (100%) | 188 (99%)  | 2 (1%)   | 65          | 74  |
| 63  | Ac    | 54/54 (100%)   | 54 (100%)  | 0        | 100         | 100 |
| 64  | AW    | 113/113 (100%) | 112 (99%)  | 1 (1%)   | 70          | 77  |
| 65  | CW    | 52/52 (100%)   | 51 (98%)   | 1 (2%)   | 50          | 66  |
| 66  | Cg    | 96/96 (100%)   | 95 (99%)   | 1 (1%)   | 68          | 76  |
| 67  | CU    | 90/90 (100%)   | 90 (100%)  | 0        | 100         | 100 |
| 68  | AK    | 81/81 (100%)   | 81 (100%)  | 0        | 100         | 100 |
| 69  | AT    | 107/116 (92%)  | 107 (100%) | 0        | 100         | 100 |
| 70  | AF    | 160/160 (100%) | 159 (99%)  | 1 (1%)   | 78          | 81  |
| 71  | CF    | 200/200 (100%) | 196 (98%)  | 4 (2%)   | 48          | 66  |
| 72  | AE    | 220/220 (100%) | 220 (100%) | 0        | 100         | 100 |
| 73  | AG    | 200/200 (100%) | 199 (100%) | 1 (0%)   | 81          | 82  |
| 74  | AH    | 175/175 (100%) | 174 (99%)  | 1 (1%)   | 78          | 81  |

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| Mol | Chain | Analysed           | Rotameric  | Outliers | Percentiles |    |
|-----|-------|--------------------|------------|----------|-------------|----|
| 75  | AI    | 175/175 (100%)     | 173 (99%)  | 2 (1%)   | 65          | 74 |
| 76  | AQ    | 122/122 (100%)     | 121 (99%)  | 1 (1%)   | 73          | 78 |
| 77  | CO    | 175/175 (100%)     | 171 (98%)  | 4 (2%)   | 44          | 63 |
| 78  | CL    | 173/173 (100%)     | 169 (98%)  | 4 (2%)   | 44          | 63 |
| 79  | CV    | 101/101 (100%)     | 98 (97%)   | 3 (3%)   | 36          | 57 |
| 80  | CM    | 138/138 (100%)     | 137 (99%)  | 1 (1%)   | 76          | 79 |
| 83  | Cj    | 71/71 (100%)       | 41 (58%)   | 30 (42%) | 0           | 0  |
| All | All   | 10126/10136 (100%) | 9981 (99%) | 145 (1%) | 57          | 72 |

All (145) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AA    | 74  | ILE  |
| 2   | CA    | 15  | VAL  |
| 2   | CA    | 136 | VAL  |
| 2   | CA    | 219 | ILE  |
| 2   | CA    | 237 | LEU  |
| 2   | CA    | 243 | THR  |
| 3   | AB    | 44  | ILE  |
| 4   | CB    | 40  | PRO  |
| 4   | CB    | 140 | ASP  |
| 4   | CB    | 223 | THR  |
| 4   | CB    | 245 | HIS  |
| 4   | CB    | 258 | HIS  |
| 4   | CB    | 278 | THR  |
| 4   | CB    | 326 | VAL  |
| 6   | CC    | 5   | ASN  |
| 6   | CC    | 14  | THR  |
| 6   | CC    | 59  | GLU  |
| 6   | CC    | 72  | THR  |
| 6   | CC    | 95  | PHE  |
| 6   | CC    | 110 | THR  |
| 6   | CC    | 304 | VAL  |
| 6   | CC    | 331 | LEU  |
| 7   | Ag    | 65  | HIS  |
| 7   | Ag    | 120 | GLN  |
| 7   | Ag    | 290 | LEU  |
| 9   | AO    | 62  | VAL  |
| 9   | AO    | 103 | ASN  |
| 10  | AX    | 26  | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13  | Ad    | 16  | GLN  |
| 14  | AN    | 56  | ASP  |
| 14  | AN    | 90  | HIS  |
| 15  | AL    | 142 | VAL  |
| 16  | AR    | 61  | LEU  |
| 17  | AP    | 8   | ASN  |
| 20  | AZ    | 47  | VAL  |
| 21  | Aa    | 40  | VAL  |
| 22  | Ab    | 53  | VAL  |
| 26  | AJ    | 74  | GLN  |
| 26  | AJ    | 149 | VAL  |
| 27  | Ca    | 44  | ILE  |
| 27  | Ca    | 45  | ASN  |
| 28  | CN    | 11  | TYR  |
| 28  | CN    | 66  | VAL  |
| 29  | CI    | 12  | CYS  |
| 29  | CI    | 196 | ASN  |
| 30  | CD    | 84  | PRO  |
| 31  | CQ    | 5   | ILE  |
| 31  | CQ    | 82  | VAL  |
| 31  | CQ    | 86  | VAL  |
| 31  | CQ    | 88  | ASP  |
| 32  | CR    | 15  | LEU  |
| 32  | CR    | 93  | LEU  |
| 32  | CR    | 143 | HIS  |
| 32  | CR    | 166 | VAL  |
| 33  | CS    | 12  | VAL  |
| 33  | CS    | 125 | GLN  |
| 34  | CT    | 7   | TYR  |
| 34  | CT    | 148 | ILE  |
| 35  | CP    | 24  | VAL  |
| 35  | CP    | 64  | ASN  |
| 35  | CP    | 119 | VAL  |
| 36  | CX    | 172 | THR  |
| 37  | CY    | 70  | VAL  |
| 37  | CY    | 101 | PRO  |
| 39  | Cr    | 9   | TRP  |
| 40  | Ch    | 101 | ASN  |
| 40  | Ch    | 121 | VAL  |
| 42  | Cc    | 51  | ASN  |
| 42  | Cc    | 96  | ILE  |
| 43  | Cd    | 56  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 43  | Cd    | 77  | THR  |
| 44  | Ce    | 25  | ASP  |
| 44  | Ce    | 52  | TYR  |
| 44  | Ce    | 57  | ILE  |
| 44  | Ce    | 91  | ASN  |
| 45  | Cf    | 12  | PRO  |
| 45  | Cf    | 47  | HIS  |
| 45  | Cf    | 107 | HIS  |
| 45  | Cf    | 138 | ASN  |
| 46  | Ci    | 11  | LEU  |
| 46  | Ci    | 43  | GLN  |
| 51  | Cp    | 51  | VAL  |
| 53  | CJ    | 79  | VAL  |
| 54  | CH    | 10  | VAL  |
| 55  | CE    | 124 | LEU  |
| 55  | CE    | 193 | VAL  |
| 55  | CE    | 227 | GLN  |
| 56  | CG    | 46  | ILE  |
| 60  | Cz    | 120 | ILE  |
| 60  | Cz    | 197 | ASN  |
| 64  | AW    | 103 | VAL  |
| 65  | CW    | 49  | VAL  |
| 66  | Cg    | 34  | TYR  |
| 70  | AF    | 158 | VAL  |
| 71  | CF    | 126 | ILE  |
| 71  | CF    | 132 | THR  |
| 71  | CF    | 144 | THR  |
| 71  | CF    | 193 | ASP  |
| 73  | AG    | 65  | GLN  |
| 74  | AH    | 150 | GLN  |
| 75  | AI    | 95  | THR  |
| 75  | AI    | 97  | VAL  |
| 76  | AQ    | 86  | ILE  |
| 77  | CO    | 37  | VAL  |
| 77  | CO    | 48  | HIS  |
| 77  | CO    | 122 | VAL  |
| 77  | CO    | 200 | SER  |
| 78  | CL    | 6   | ASN  |
| 78  | CL    | 69  | LEU  |
| 78  | CL    | 75  | PHE  |
| 78  | CL    | 148 | GLN  |
| 79  | CV    | 30  | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 79  | CV    | 64  | THR  |
| 79  | CV    | 80  | VAL  |
| 80  | CM    | 110 | PHE  |
| 83  | Cj    | 2   | THR  |
| 83  | Cj    | 3   | LYS  |
| 83  | Cj    | 7   | SER  |
| 83  | Cj    | 10  | LYS  |
| 83  | Cj    | 13  | ASN  |
| 83  | Cj    | 14  | LYS  |
| 83  | Cj    | 16  | HIS  |
| 83  | Cj    | 18  | ILE  |
| 83  | Cj    | 19  | CYS  |
| 83  | Cj    | 21  | ARG  |
| 83  | Cj    | 24  | ASN  |
| 83  | Cj    | 25  | SER  |
| 83  | Cj    | 31  | LYS  |
| 83  | Cj    | 33  | LYS  |
| 83  | Cj    | 37  | CYS  |
| 83  | Cj    | 43  | LYS  |
| 83  | Cj    | 45  | ARG  |
| 83  | Cj    | 46  | SER  |
| 83  | Cj    | 50  | SER  |
| 83  | Cj    | 51  | ARG  |
| 83  | Cj    | 52  | LYS  |
| 83  | Cj    | 54  | LYS  |
| 83  | Cj    | 56  | ARG  |
| 83  | Cj    | 61  | THR  |
| 83  | Cj    | 65  | ARG  |
| 83  | Cj    | 70  | LEU  |
| 83  | Cj    | 71  | ARG  |
| 83  | Cj    | 72  | ARG  |
| 83  | Cj    | 73  | ARG  |
| 83  | Cj    | 74  | PHE  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (99) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AA    | 50  | ASN  |
| 1   | AA    | 141 | ASN  |
| 1   | AA    | 164 | ASN  |
| 2   | CA    | 106 | GLN  |
| 3   | AB    | 75  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | AB    | 161 | GLN  |
| 4   | CB    | 173 | GLN  |
| 4   | CB    | 186 | ASN  |
| 4   | CB    | 281 | ASN  |
| 5   | AC    | 119 | HIS  |
| 6   | CC    | 53  | GLN  |
| 6   | CC    | 97  | ASN  |
| 6   | CC    | 284 | GLN  |
| 7   | Ag    | 52  | ASN  |
| 7   | Ag    | 189 | HIS  |
| 9   | AO    | 20  | GLN  |
| 10  | AX    | 39  | ASN  |
| 11  | AM    | 26  | GLN  |
| 11  | AM    | 89  | HIS  |
| 13  | Ad    | 48  | ASN  |
| 14  | AN    | 5   | HIS  |
| 14  | AN    | 67  | ASN  |
| 15  | AL    | 4   | GLN  |
| 16  | AR    | 118 | GLN  |
| 17  | AP    | 33  | ASN  |
| 19  | AY    | 16  | ASN  |
| 19  | AY    | 64  | ASN  |
| 19  | AY    | 113 | ASN  |
| 20  | AZ    | 45  | ASN  |
| 23  | AD    | 147 | GLN  |
| 24  | Ae    | 94  | GLN  |
| 26  | AJ    | 141 | GLN  |
| 26  | AJ    | 183 | GLN  |
| 27  | Ca    | 35  | ASN  |
| 27  | Ca    | 45  | ASN  |
| 28  | CN    | 87  | HIS  |
| 30  | CD    | 9   | ASN  |
| 30  | CD    | 45  | ASN  |
| 30  | CD    | 245 | GLN  |
| 31  | CQ    | 104 | HIS  |
| 31  | CQ    | 107 | GLN  |
| 32  | CR    | 118 | HIS  |
| 32  | CR    | 143 | HIS  |
| 34  | CT    | 22  | HIS  |
| 34  | CT    | 45  | HIS  |
| 34  | CT    | 49  | GLN  |
| 35  | CP    | 28  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 35  | CP    | 178 | GLN  |
| 36  | CX    | 164 | ASN  |
| 36  | CX    | 214 | ASN  |
| 37  | CY    | 3   | GLN  |
| 40  | Ch    | 68  | ASN  |
| 44  | Ce    | 32  | HIS  |
| 44  | Ce    | 67  | HIS  |
| 44  | Ce    | 79  | HIS  |
| 45  | Cf    | 69  | ASN  |
| 46  | Ci    | 102 | ASN  |
| 48  | Cl    | 19  | GLN  |
| 49  | Cm    | 90  | ASN  |
| 52  | Co    | 3   | ASN  |
| 52  | Co    | 51  | GLN  |
| 53  | CJ    | 52  | GLN  |
| 54  | CH    | 5   | ASN  |
| 54  | CH    | 77  | ASN  |
| 55  | CE    | 162 | HIS  |
| 55  | CE    | 197 | GLN  |
| 56  | CG    | 51  | GLN  |
| 56  | CG    | 230 | ASN  |
| 60  | Cz    | 94  | ASN  |
| 60  | Cz    | 96  | ASN  |
| 60  | Cz    | 182 | ASN  |
| 60  | Cz    | 197 | ASN  |
| 63  | Ac    | 41  | ASN  |
| 64  | AW    | 24  | GLN  |
| 64  | AW    | 64  | ASN  |
| 66  | Cg    | 46  | GLN  |
| 68  | AK    | 59  | GLN  |
| 69  | AT    | 63  | HIS  |
| 69  | AT    | 85  | ASN  |
| 69  | AT    | 88  | HIS  |
| 69  | AT    | 128 | GLN  |
| 71  | CF    | 149 | ASN  |
| 71  | CF    | 229 | ASN  |
| 71  | CF    | 239 | ASN  |
| 72  | AE    | 36  | HIS  |
| 72  | AE    | 57  | ASN  |
| 73  | AG    | 56  | ASN  |
| 73  | AG    | 65  | GLN  |
| 73  | AG    | 216 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 74  | AH    | 74  | GLN  |
| 74  | AH    | 89  | HIS  |
| 76  | AQ    | 13  | GLN  |
| 77  | CO    | 44  | ASN  |
| 77  | CO    | 52  | ASN  |
| 77  | CO    | 195 | ASN  |
| 78  | CL    | 88  | ASN  |
| 80  | CM    | 33  | GLN  |
| 80  | CM    | 118 | GLN  |
| 83  | Cj    | 30  | GLN  |

### 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 57  | A9    | 29/30 (96%)     | 10 (34%)          | 1 (3%)          |
| 58  | A7    | 119/120 (99%)   | 30 (25%)          | 1 (0%)          |
| 59  | A8    | 122/123 (99%)   | 58 (47%)          | 2 (1%)          |
| 61  | B2    | 1787/1995 (89%) | 723 (40%)         | 26 (1%)         |
| 62  | A5    | 3560/3974 (89%) | 1649 (46%)        | 86 (2%)         |
| 81  | B     | 74/75 (98%)     | 27 (36%)          | 1 (1%)          |
| 82  | v     | 11/12 (91%)     | 6 (54%)           | 0               |
| All | All   | 5702/6329 (90%) | 2503 (43%)        | 117 (2%)        |

All (2503) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 57  | A9    | 7   | G    |
| 57  | A9    | 9   | C    |
| 57  | A9    | 10  | U    |
| 57  | A9    | 11  | A    |
| 57  | A9    | 15  | A    |
| 57  | A9    | 16  | U    |
| 57  | A9    | 21  | G    |
| 57  | A9    | 22  | A    |
| 57  | A9    | 24  | G    |
| 57  | A9    | 30  | A    |
| 58  | A7    | 2   | C    |
| 58  | A7    | 10  | C    |
| 58  | A7    | 11  | A    |
| 58  | A7    | 21  | G    |
| 58  | A7    | 22  | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 58  | A7    | 25  | A    |
| 58  | A7    | 27  | A    |
| 58  | A7    | 33  | U    |
| 58  | A7    | 38  | U    |
| 58  | A7    | 50  | A    |
| 58  | A7    | 60  | C    |
| 58  | A7    | 61  | G    |
| 58  | A7    | 62  | U    |
| 58  | A7    | 64  | G    |
| 58  | A7    | 66  | G    |
| 58  | A7    | 72  | U    |
| 58  | A7    | 74  | A    |
| 58  | A7    | 76  | U    |
| 58  | A7    | 86  | G    |
| 58  | A7    | 88  | G    |
| 58  | A7    | 92  | C    |
| 58  | A7    | 94  | C    |
| 58  | A7    | 97  | G    |
| 58  | A7    | 100 | A    |
| 58  | A7    | 103 | A    |
| 58  | A7    | 108 | G    |
| 58  | A7    | 109 | U    |
| 58  | A7    | 110 | G    |
| 58  | A7    | 112 | U    |
| 58  | A7    | 120 | U    |
| 59  | A8    | 2   | A    |
| 59  | A8    | 8   | A    |
| 59  | A8    | 13  | U    |
| 59  | A8    | 14  | G    |
| 59  | A8    | 15  | G    |
| 59  | A8    | 18  | C    |
| 59  | A8    | 19  | A    |
| 59  | A8    | 20  | C    |
| 59  | A8    | 21  | U    |
| 59  | A8    | 22  | C    |
| 59  | A8    | 23  | G    |
| 59  | A8    | 24  | G    |
| 59  | A8    | 25  | C    |
| 59  | A8    | 30  | G    |
| 59  | A8    | 31  | G    |
| 59  | A8    | 32  | G    |
| 59  | A8    | 33  | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 59  | A8    | 34  | C    |
| 59  | A8    | 35  | G    |
| 59  | A8    | 38  | G    |
| 59  | A8    | 41  | G    |
| 59  | A8    | 46  | C    |
| 59  | A8    | 48  | G    |
| 59  | A8    | 50  | A    |
| 59  | A8    | 52  | A    |
| 59  | A8    | 53  | C    |
| 59  | A8    | 56  | U    |
| 59  | A8    | 57  | G    |
| 59  | A8    | 59  | G    |
| 59  | A8    | 60  | U    |
| 59  | A8    | 61  | C    |
| 59  | A8    | 62  | A    |
| 59  | A8    | 69  | G    |
| 59  | A8    | 70  | A    |
| 59  | A8    | 80  | C    |
| 59  | A8    | 81  | A    |
| 59  | A8    | 83  | A    |
| 59  | A8    | 84  | U    |
| 59  | A8    | 85  | G    |
| 59  | A8    | 86  | A    |
| 59  | A8    | 92  | G    |
| 59  | A8    | 94  | C    |
| 59  | A8    | 95  | A    |
| 59  | A8    | 99  | U    |
| 59  | A8    | 100 | G    |
| 59  | A8    | 101 | A    |
| 59  | A8    | 102 | A    |
| 59  | A8    | 103 | C    |
| 59  | A8    | 104 | G    |
| 59  | A8    | 106 | A    |
| 59  | A8    | 107 | U    |
| 59  | A8    | 108 | A    |
| 59  | A8    | 109 | U    |
| 59  | A8    | 110 | C    |
| 59  | A8    | 113 | A    |
| 59  | A8    | 117 | C    |
| 59  | A8    | 122 | U    |
| 59  | A8    | 123 | G    |
| 61  | B2    | 2   | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 61  | B2    | 4   | C    |
| 61  | B2    | 25  | U    |
| 61  | B2    | 26  | A    |
| 61  | B2    | 27  | U    |
| 61  | B2    | 34  | G    |
| 61  | B2    | 36  | C    |
| 61  | B2    | 38  | C    |
| 61  | B2    | 42  | G    |
| 61  | B2    | 46  | A    |
| 61  | B2    | 47  | A    |
| 61  | B2    | 56  | U    |
| 61  | B2    | 57  | G    |
| 61  | B2    | 65  | A    |
| 61  | B2    | 66  | C    |
| 61  | B2    | 68  | C    |
| 61  | B2    | 69  | A    |
| 61  | B2    | 70  | C    |
| 61  | B2    | 73  | A    |
| 61  | B2    | 74  | U    |
| 61  | B2    | 75  | U    |
| 61  | B2    | 76  | A    |
| 61  | B2    | 77  | A    |
| 61  | B2    | 80  | G    |
| 61  | B2    | 82  | G    |
| 61  | B2    | 83  | A    |
| 61  | B2    | 84  | A    |
| 61  | B2    | 98  | C    |
| 61  | B2    | 99  | A    |
| 61  | B2    | 100 | U    |
| 61  | B2    | 101 | U    |
| 61  | B2    | 103 | U    |
| 61  | B2    | 104 | A    |
| 61  | B2    | 108 | G    |
| 61  | B2    | 110 | U    |
| 61  | B2    | 111 | A    |
| 61  | B2    | 113 | G    |
| 61  | B2    | 114 | G    |
| 61  | B2    | 115 | U    |
| 61  | B2    | 121 | A    |
| 61  | B2    | 122 | G    |
| 61  | B2    | 123 | A    |
| 61  | B2    | 124 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 61  | B2    | 125 | C    |
| 61  | B2    | 126 | G    |
| 61  | B2    | 136 | A    |
| 61  | B2    | 137 | C    |
| 61  | B2    | 138 | U    |
| 61  | B2    | 139 | U    |
| 61  | B2    | 141 | G    |
| 61  | B2    | 142 | A    |
| 61  | B2    | 143 | U    |
| 61  | B2    | 145 | A    |
| 61  | B2    | 150 | G    |
| 61  | B2    | 152 | U    |
| 61  | B2    | 153 | A    |
| 61  | B2    | 155 | U    |
| 61  | B2    | 156 | U    |
| 61  | B2    | 163 | C    |
| 61  | B2    | 167 | U    |
| 61  | B2    | 172 | G    |
| 61  | B2    | 173 | C    |
| 61  | B2    | 174 | A    |
| 61  | B2    | 177 | U    |
| 61  | B2    | 178 | A    |
| 61  | B2    | 183 | A    |
| 61  | B2    | 184 | U    |
| 61  | B2    | 185 | G    |
| 61  | B2    | 188 | C    |
| 61  | B2    | 190 | U    |
| 61  | B2    | 191 | U    |
| 61  | B2    | 193 | U    |
| 61  | B2    | 194 | G    |
| 61  | B2    | 200 | U    |
| 61  | B2    | 203 | G    |
| 61  | B2    | 205 | U    |
| 61  | B2    | 210 | U    |
| 61  | B2    | 214 | G    |
| 61  | B2    | 215 | C    |
| 61  | B2    | 216 | U    |
| 61  | B2    | 224 | A    |
| 61  | B2    | 226 | C    |
| 61  | B2    | 227 | G    |
| 61  | B2    | 233 | A    |
| 61  | B2    | 234 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 61  | B2    | 235 | G    |
| 61  | B2    | 236 | A    |
| 61  | B2    | 238 | C    |
| 61  | B2    | 249 | U    |
| 61  | B2    | 250 | U    |
| 61  | B2    | 251 | G    |
| 61  | B2    | 252 | A    |
| 61  | B2    | 253 | A    |
| 61  | B2    | 254 | C    |
| 61  | B2    | 255 | U    |
| 61  | B2    | 256 | C    |
| 61  | B2    | 257 | U    |
| 61  | B2    | 258 | A    |
| 61  | B2    | 259 | G    |
| 61  | B2    | 263 | A    |
| 61  | B2    | 266 | U    |
| 61  | B2    | 267 | G    |
| 61  | B2    | 270 | G    |
| 61  | B2    | 276 | A    |
| 61  | B2    | 279 | G    |
| 61  | B2    | 281 | C    |
| 61  | B2    | 282 | U    |
| 61  | B2    | 283 | U    |
| 61  | B2    | 284 | G    |
| 61  | B2    | 285 | U    |
| 61  | B2    | 289 | G    |
| 61  | B2    | 290 | A    |
| 61  | B2    | 291 | C    |
| 61  | B2    | 292 | G    |
| 61  | B2    | 293 | A    |
| 61  | B2    | 294 | C    |
| 61  | B2    | 302 | U    |
| 61  | B2    | 304 | A    |
| 61  | B2    | 313 | C    |
| 61  | B2    | 317 | A    |
| 61  | B2    | 319 | C    |
| 61  | B2    | 321 | A    |
| 61  | B2    | 322 | C    |
| 61  | B2    | 324 | U    |
| 61  | B2    | 325 | U    |
| 61  | B2    | 326 | U    |
| 61  | B2    | 327 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 61  | B2    | 330 | G    |
| 61  | B2    | 336 | A    |
| 61  | B2    | 338 | C    |
| 61  | B2    | 339 | U    |
| 61  | B2    | 341 | G    |
| 61  | B2    | 342 | G    |
| 61  | B2    | 343 | A    |
| 61  | B2    | 347 | C    |
| 61  | B2    | 352 | G    |
| 61  | B2    | 357 | A    |
| 61  | B2    | 358 | A    |
| 61  | B2    | 359 | C    |
| 61  | B2    | 361 | G    |
| 61  | B2    | 364 | A    |
| 61  | B2    | 365 | A    |
| 61  | B2    | 366 | C    |
| 61  | B2    | 370 | G    |
| 61  | B2    | 373 | U    |
| 61  | B2    | 375 | A    |
| 61  | B2    | 376 | G    |
| 61  | B2    | 379 | U    |
| 61  | B2    | 380 | U    |
| 61  | B2    | 381 | C    |
| 61  | B2    | 382 | G    |
| 61  | B2    | 383 | A    |
| 61  | B2    | 385 | U    |
| 61  | B2    | 386 | C    |
| 61  | B2    | 390 | A    |
| 61  | B2    | 392 | A    |
| 61  | B2    | 395 | G    |
| 61  | B2    | 397 | G    |
| 61  | B2    | 402 | A    |
| 61  | B2    | 404 | A    |
| 61  | B2    | 405 | A    |
| 61  | B2    | 406 | A    |
| 61  | B2    | 407 | C    |
| 61  | B2    | 408 | G    |
| 61  | B2    | 409 | G    |
| 61  | B2    | 413 | C    |
| 61  | B2    | 417 | A    |
| 61  | B2    | 420 | U    |
| 61  | B2    | 421 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 61  | B2    | 422 | A    |
| 61  | B2    | 423 | G    |
| 61  | B2    | 428 | G    |
| 61  | B2    | 429 | C    |
| 61  | B2    | 430 | A    |
| 61  | B2    | 431 | G    |
| 61  | B2    | 434 | G    |
| 61  | B2    | 441 | A    |
| 61  | B2    | 444 | U    |
| 61  | B2    | 449 | C    |
| 61  | B2    | 450 | A    |
| 61  | B2    | 453 | C    |
| 61  | B2    | 457 | G    |
| 61  | B2    | 464 | G    |
| 61  | B2    | 466 | G    |
| 61  | B2    | 472 | G    |
| 61  | B2    | 474 | C    |
| 61  | B2    | 475 | G    |
| 61  | B2    | 476 | A    |
| 61  | B2    | 482 | A    |
| 61  | B2    | 489 | C    |
| 61  | B2    | 490 | A    |
| 61  | B2    | 501 | C    |
| 61  | B2    | 506 | G    |
| 61  | B2    | 508 | C    |
| 61  | B2    | 509 | C    |
| 61  | B2    | 510 | U    |
| 61  | B2    | 511 | G    |
| 61  | B2    | 512 | U    |
| 61  | B2    | 513 | A    |
| 61  | B2    | 514 | A    |
| 61  | B2    | 515 | U    |
| 61  | B2    | 516 | U    |
| 61  | B2    | 517 | G    |
| 61  | B2    | 519 | A    |
| 61  | B2    | 521 | U    |
| 61  | B2    | 522 | G    |
| 61  | B2    | 523 | A    |
| 61  | B2    | 524 | G    |
| 61  | B2    | 527 | C    |
| 61  | B2    | 541 | U    |
| 61  | B2    | 542 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 61  | B2    | 546 | A    |
| 61  | B2    | 547 | G    |
| 61  | B2    | 548 | G    |
| 61  | B2    | 549 | A    |
| 61  | B2    | 550 | C    |
| 61  | B2    | 551 | C    |
| 61  | B2    | 553 | A    |
| 61  | B2    | 554 | U    |
| 61  | B2    | 563 | A    |
| 61  | B2    | 564 | A    |
| 61  | B2    | 565 | G    |
| 61  | B2    | 566 | U    |
| 61  | B2    | 567 | C    |
| 61  | B2    | 572 | G    |
| 61  | B2    | 573 | C    |
| 61  | B2    | 576 | G    |
| 61  | B2    | 582 | G    |
| 61  | B2    | 586 | U    |
| 61  | B2    | 587 | A    |
| 61  | B2    | 588 | A    |
| 61  | B2    | 589 | U    |
| 61  | B2    | 593 | A    |
| 61  | B2    | 602 | A    |
| 61  | B2    | 603 | G    |
| 61  | B2    | 609 | A    |
| 61  | B2    | 613 | A    |
| 61  | B2    | 614 | A    |
| 61  | B2    | 616 | U    |
| 61  | B2    | 617 | U    |
| 61  | B2    | 619 | U    |
| 61  | B2    | 620 | U    |
| 61  | B2    | 625 | U    |
| 61  | B2    | 627 | A    |
| 61  | B2    | 628 | A    |
| 61  | B2    | 631 | C    |
| 61  | B2    | 632 | G    |
| 61  | B2    | 633 | U    |
| 61  | B2    | 637 | U    |
| 61  | B2    | 639 | G    |
| 61  | B2    | 643 | A    |
| 61  | B2    | 646 | U    |
| 61  | B2    | 647 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 61  | B2    | 649 | U    |
| 61  | B2    | 655 | A    |
| 61  | B2    | 656 | U    |
| 61  | B2    | 706 | U    |
| 61  | B2    | 713 | A    |
| 61  | B2    | 714 | U    |
| 61  | B2    | 715 | U    |
| 61  | B2    | 719 | G    |
| 61  | B2    | 819 | G    |
| 61  | B2    | 821 | U    |
| 61  | B2    | 824 | U    |
| 61  | B2    | 825 | A    |
| 61  | B2    | 826 | U    |
| 61  | B2    | 833 | G    |
| 61  | B2    | 837 | A    |
| 61  | B2    | 843 | G    |
| 61  | B2    | 844 | A    |
| 61  | B2    | 847 | G    |
| 61  | B2    | 848 | C    |
| 61  | B2    | 853 | A    |
| 61  | B2    | 856 | A    |
| 61  | B2    | 857 | G    |
| 61  | B2    | 860 | U    |
| 61  | B2    | 861 | U    |
| 61  | B2    | 862 | C    |
| 61  | B2    | 863 | A    |
| 61  | B2    | 864 | A    |
| 61  | B2    | 865 | A    |
| 61  | B2    | 866 | U    |
| 61  | B2    | 867 | G    |
| 61  | B2    | 868 | C    |
| 61  | B2    | 869 | C    |
| 61  | B2    | 871 | G    |
| 61  | B2    | 873 | A    |
| 61  | B2    | 875 | A    |
| 61  | B2    | 876 | U    |
| 61  | B2    | 877 | U    |
| 61  | B2    | 878 | C    |
| 61  | B2    | 879 | U    |
| 61  | B2    | 880 | G    |
| 61  | B2    | 881 | U    |
| 61  | B2    | 888 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 61  | B2    | 892 | A    |
| 61  | B2    | 895 | A    |
| 61  | B2    | 897 | A    |
| 61  | B2    | 899 | A    |
| 61  | B2    | 900 | A    |
| 61  | B2    | 901 | G    |
| 61  | B2    | 902 | A    |
| 61  | B2    | 903 | C    |
| 61  | B2    | 905 | U    |
| 61  | B2    | 907 | U    |
| 61  | B2    | 908 | G    |
| 61  | B2    | 909 | U    |
| 61  | B2    | 910 | U    |
| 61  | B2    | 911 | C    |
| 61  | B2    | 913 | G    |
| 61  | B2    | 914 | C    |
| 61  | B2    | 915 | U    |
| 61  | B2    | 916 | U    |
| 61  | B2    | 918 | C    |
| 61  | B2    | 919 | A    |
| 61  | B2    | 920 | U    |
| 61  | B2    | 922 | G    |
| 61  | B2    | 926 | U    |
| 61  | B2    | 929 | A    |
| 61  | B2    | 930 | G    |
| 61  | B2    | 933 | C    |
| 61  | B2    | 935 | A    |
| 61  | B2    | 937 | A    |
| 61  | B2    | 938 | G    |
| 61  | B2    | 939 | G    |
| 61  | B2    | 940 | U    |
| 61  | B2    | 941 | A    |
| 61  | B2    | 942 | A    |
| 61  | B2    | 943 | U    |
| 61  | B2    | 944 | G    |
| 61  | B2    | 946 | U    |
| 61  | B2    | 949 | A    |
| 61  | B2    | 950 | U    |
| 61  | B2    | 957 | A    |
| 61  | B2    | 958 | G    |
| 61  | B2    | 959 | U    |
| 61  | B2    | 960 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 61  | B2    | 961  | U    |
| 61  | B2    | 963  | G    |
| 61  | B2    | 973  | U    |
| 61  | B2    | 974  | A    |
| 61  | B2    | 975  | U    |
| 61  | B2    | 977  | A    |
| 61  | B2    | 993  | A    |
| 61  | B2    | 998  | U    |
| 61  | B2    | 999  | U    |
| 61  | B2    | 1000 | G    |
| 61  | B2    | 1002 | A    |
| 61  | B2    | 1005 | G    |
| 61  | B2    | 1010 | A    |
| 61  | B2    | 1017 | A    |
| 61  | B2    | 1018 | C    |
| 61  | B2    | 1019 | U    |
| 61  | B2    | 1020 | U    |
| 61  | B2    | 1021 | A    |
| 61  | B2    | 1022 | A    |
| 61  | B2    | 1029 | G    |
| 61  | B2    | 1031 | A    |
| 61  | B2    | 1032 | U    |
| 61  | B2    | 1037 | C    |
| 61  | B2    | 1038 | A    |
| 61  | B2    | 1040 | A    |
| 61  | B2    | 1047 | U    |
| 61  | B2    | 1050 | A    |
| 61  | B2    | 1053 | A    |
| 61  | B2    | 1057 | A    |
| 61  | B2    | 1058 | A    |
| 61  | B2    | 1059 | G    |
| 61  | B2    | 1070 | A    |
| 61  | B2    | 1072 | A    |
| 61  | B2    | 1074 | G    |
| 61  | B2    | 1079 | A    |
| 61  | B2    | 1080 | A    |
| 61  | B2    | 1082 | G    |
| 61  | B2    | 1090 | A    |
| 61  | B2    | 1091 | U    |
| 61  | B2    | 1092 | A    |
| 61  | B2    | 1094 | C    |
| 61  | B2    | 1096 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 61  | B2    | 1098 | C    |
| 61  | B2    | 1101 | G    |
| 61  | B2    | 1107 | A    |
| 61  | B2    | 1108 | C    |
| 61  | B2    | 1110 | A    |
| 61  | B2    | 1111 | U    |
| 61  | B2    | 1112 | A    |
| 61  | B2    | 1113 | A    |
| 61  | B2    | 1114 | A    |
| 61  | B2    | 1115 | C    |
| 61  | B2    | 1117 | A    |
| 61  | B2    | 1118 | U    |
| 61  | B2    | 1119 | G    |
| 61  | B2    | 1126 | A    |
| 61  | B2    | 1127 | G    |
| 61  | B2    | 1133 | G    |
| 61  | B2    | 1138 | U    |
| 61  | B2    | 1139 | A    |
| 61  | B2    | 1140 | G    |
| 61  | B2    | 1144 | C    |
| 61  | B2    | 1145 | U    |
| 61  | B2    | 1148 | U    |
| 61  | B2    | 1150 | U    |
| 61  | B2    | 1159 | C    |
| 61  | B2    | 1161 | G    |
| 61  | B2    | 1164 | G    |
| 61  | B2    | 1167 | U    |
| 61  | B2    | 1168 | C    |
| 61  | B2    | 1169 | C    |
| 61  | B2    | 1170 | G    |
| 61  | B2    | 1172 | G    |
| 61  | B2    | 1174 | A    |
| 61  | B2    | 1175 | A    |
| 61  | B2    | 1178 | A    |
| 61  | B2    | 1179 | A    |
| 61  | B2    | 1180 | A    |
| 61  | B2    | 1183 | U    |
| 61  | B2    | 1184 | U    |
| 61  | B2    | 1185 | U    |
| 61  | B2    | 1186 | U    |
| 61  | B2    | 1187 | U    |
| 61  | B2    | 1188 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 61  | B2    | 1189 | G    |
| 61  | B2    | 1190 | G    |
| 61  | B2    | 1193 | C    |
| 61  | B2    | 1197 | G    |
| 61  | B2    | 1198 | G    |
| 61  | B2    | 1199 | G    |
| 61  | B2    | 1200 | A    |
| 61  | B2    | 1201 | A    |
| 61  | B2    | 1206 | G    |
| 61  | B2    | 1207 | G    |
| 61  | B2    | 1217 | U    |
| 61  | B2    | 1218 | G    |
| 61  | B2    | 1220 | A    |
| 61  | B2    | 1221 | A    |
| 61  | B2    | 1226 | A    |
| 61  | B2    | 1230 | A    |
| 61  | B2    | 1234 | G    |
| 61  | B2    | 1236 | C    |
| 61  | B2    | 1238 | G    |
| 61  | B2    | 1239 | A    |
| 61  | B2    | 1240 | A    |
| 61  | B2    | 1244 | C    |
| 61  | B2    | 1245 | A    |
| 61  | B2    | 1246 | C    |
| 61  | B2    | 1247 | C    |
| 61  | B2    | 1248 | A    |
| 61  | B2    | 1251 | A    |
| 61  | B2    | 1252 | G    |
| 61  | B2    | 1255 | G    |
| 61  | B2    | 1260 | G    |
| 61  | B2    | 1263 | U    |
| 61  | B2    | 1265 | C    |
| 61  | B2    | 1273 | U    |
| 61  | B2    | 1278 | C    |
| 61  | B2    | 1279 | U    |
| 61  | B2    | 1281 | A    |
| 61  | B2    | 1282 | A    |
| 61  | B2    | 1283 | C    |
| 61  | B2    | 1284 | A    |
| 61  | B2    | 1285 | C    |
| 61  | B2    | 1287 | G    |
| 61  | B2    | 1288 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 61  | B2    | 1289 | A    |
| 61  | B2    | 1290 | A    |
| 61  | B2    | 1292 | A    |
| 61  | B2    | 1294 | U    |
| 61  | B2    | 1301 | G    |
| 61  | B2    | 1305 | A    |
| 61  | B2    | 1306 | A    |
| 61  | B2    | 1307 | C    |
| 61  | B2    | 1309 | U    |
| 61  | B2    | 1310 | A    |
| 61  | B2    | 1311 | A    |
| 61  | B2    | 1313 | U    |
| 61  | B2    | 1314 | G    |
| 61  | B2    | 1316 | G    |
| 61  | B2    | 1317 | U    |
| 61  | B2    | 1318 | A    |
| 61  | B2    | 1321 | A    |
| 61  | B2    | 1324 | G    |
| 61  | B2    | 1325 | A    |
| 61  | B2    | 1327 | U    |
| 61  | B2    | 1328 | G    |
| 61  | B2    | 1330 | U    |
| 61  | B2    | 1335 | C    |
| 61  | B2    | 1339 | C    |
| 61  | B2    | 1341 | C    |
| 61  | B2    | 1342 | G    |
| 61  | B2    | 1343 | A    |
| 61  | B2    | 1346 | C    |
| 61  | B2    | 1348 | A    |
| 61  | B2    | 1349 | U    |
| 61  | B2    | 1351 | G    |
| 61  | B2    | 1352 | G    |
| 61  | B2    | 1363 | U    |
| 61  | B2    | 1371 | C    |
| 61  | B2    | 1373 | U    |
| 61  | B2    | 1374 | A    |
| 61  | B2    | 1375 | G    |
| 61  | B2    | 1379 | G    |
| 61  | B2    | 1381 | G    |
| 61  | B2    | 1382 | G    |
| 61  | B2    | 1384 | G    |
| 61  | B2    | 1385 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 61  | B2    | 1387 | A    |
| 61  | B2    | 1388 | U    |
| 61  | B2    | 1393 | C    |
| 61  | B2    | 1394 | U    |
| 61  | B2    | 1400 | A    |
| 61  | B2    | 1401 | U    |
| 61  | B2    | 1406 | A    |
| 61  | B2    | 1407 | U    |
| 61  | B2    | 1408 | A    |
| 61  | B2    | 1409 | A    |
| 61  | B2    | 1410 | C    |
| 61  | B2    | 1411 | G    |
| 61  | B2    | 1412 | A    |
| 61  | B2    | 1423 | A    |
| 61  | B2    | 1424 | A    |
| 61  | B2    | 1425 | U    |
| 61  | B2    | 1426 | A    |
| 61  | B2    | 1427 | U    |
| 61  | B2    | 1428 | A    |
| 61  | B2    | 1430 | U    |
| 61  | B2    | 1432 | A    |
| 61  | B2    | 1433 | A    |
| 61  | B2    | 1436 | G    |
| 61  | B2    | 1438 | U    |
| 61  | B2    | 1442 | U    |
| 61  | B2    | 1446 | G    |
| 61  | B2    | 1449 | U    |
| 61  | B2    | 1450 | U    |
| 61  | B2    | 1451 | A    |
| 61  | B2    | 1453 | G    |
| 61  | B2    | 1458 | U    |
| 61  | B2    | 1529 | G    |
| 61  | B2    | 1530 | A    |
| 61  | B2    | 1531 | G    |
| 61  | B2    | 1541 | U    |
| 61  | B2    | 1544 | G    |
| 61  | B2    | 1545 | U    |
| 61  | B2    | 1546 | U    |
| 61  | B2    | 1547 | U    |
| 61  | B2    | 1548 | G    |
| 61  | B2    | 1551 | C    |
| 61  | B2    | 1552 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 61  | B2    | 1557 | U    |
| 61  | B2    | 1558 | A    |
| 61  | B2    | 1561 | G    |
| 61  | B2    | 1565 | C    |
| 61  | B2    | 1566 | U    |
| 61  | B2    | 1567 | A    |
| 61  | B2    | 1569 | C    |
| 61  | B2    | 1570 | U    |
| 61  | B2    | 1571 | U    |
| 61  | B2    | 1572 | C    |
| 61  | B2    | 1575 | A    |
| 61  | B2    | 1576 | A    |
| 61  | B2    | 1578 | U    |
| 61  | B2    | 1579 | G    |
| 61  | B2    | 1581 | A    |
| 61  | B2    | 1582 | C    |
| 61  | B2    | 1584 | A    |
| 61  | B2    | 1585 | A    |
| 61  | B2    | 1588 | G    |
| 61  | B2    | 1589 | C    |
| 61  | B2    | 1591 | U    |
| 61  | B2    | 1593 | U    |
| 61  | B2    | 1594 | A    |
| 61  | B2    | 1595 | G    |
| 61  | B2    | 1596 | C    |
| 61  | B2    | 1597 | A    |
| 61  | B2    | 1599 | U    |
| 61  | B2    | 1600 | A    |
| 61  | B2    | 1601 | A    |
| 61  | B2    | 1602 | U    |
| 61  | B2    | 1603 | G    |
| 61  | B2    | 1604 | A    |
| 61  | B2    | 1605 | G    |
| 61  | B2    | 1608 | U    |
| 61  | B2    | 1609 | G    |
| 61  | B2    | 1614 | A    |
| 61  | B2    | 1615 | U    |
| 61  | B2    | 1617 | A    |
| 61  | B2    | 1619 | A    |
| 61  | B2    | 1620 | G    |
| 61  | B2    | 1623 | C    |
| 61  | B2    | 1626 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 61  | B2    | 1627 | G    |
| 61  | B2    | 1628 | A    |
| 61  | B2    | 1636 | A    |
| 61  | B2    | 1637 | G    |
| 61  | B2    | 1638 | A    |
| 61  | B2    | 1639 | U    |
| 61  | B2    | 1640 | G    |
| 61  | B2    | 1643 | C    |
| 61  | B2    | 1645 | G    |
| 61  | B2    | 1651 | C    |
| 61  | B2    | 1652 | A    |
| 61  | B2    | 1653 | C    |
| 61  | B2    | 1655 | C    |
| 61  | B2    | 1658 | G    |
| 61  | B2    | 1659 | C    |
| 61  | B2    | 1664 | A    |
| 61  | B2    | 1665 | U    |
| 61  | B2    | 1666 | G    |
| 61  | B2    | 1668 | A    |
| 61  | B2    | 1669 | A    |
| 61  | B2    | 1670 | G    |
| 61  | B2    | 1674 | C    |
| 61  | B2    | 1675 | A    |
| 61  | B2    | 1678 | G    |
| 61  | B2    | 1682 | A    |
| 61  | B2    | 1684 | U    |
| 61  | B2    | 1685 | U    |
| 61  | B2    | 1688 | U    |
| 61  | B2    | 1691 | A    |
| 61  | B2    | 1695 | A    |
| 61  | B2    | 1698 | G    |
| 61  | B2    | 1702 | C    |
| 61  | B2    | 1703 | G    |
| 61  | B2    | 1708 | A    |
| 61  | B2    | 1709 | A    |
| 61  | B2    | 1712 | G    |
| 61  | B2    | 1713 | C    |
| 61  | B2    | 1714 | U    |
| 61  | B2    | 1715 | G    |
| 61  | B2    | 1716 | A    |
| 61  | B2    | 1718 | C    |
| 61  | B2    | 1719 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 61  | B2    | 1720 | A    |
| 61  | B2    | 1723 | U    |
| 61  | B2    | 1725 | C    |
| 61  | B2    | 1726 | A    |
| 61  | B2    | 1727 | U    |
| 61  | B2    | 1729 | C    |
| 61  | B2    | 1732 | G    |
| 61  | B2    | 1734 | G    |
| 61  | B2    | 1735 | A    |
| 61  | B2    | 1742 | A    |
| 61  | B2    | 1746 | A    |
| 61  | B2    | 1748 | A    |
| 61  | B2    | 1749 | C    |
| 61  | B2    | 1750 | U    |
| 61  | B2    | 1751 | G    |
| 61  | B2    | 1752 | U    |
| 61  | B2    | 1758 | A    |
| 61  | B2    | 1765 | U    |
| 61  | B2    | 1766 | G    |
| 61  | B2    | 1775 | A    |
| 61  | B2    | 1782 | G    |
| 61  | B2    | 1788 | C    |
| 61  | B2    | 1793 | A    |
| 61  | B2    | 1794 | C    |
| 61  | B2    | 1795 | U    |
| 61  | B2    | 1796 | C    |
| 61  | B2    | 1802 | G    |
| 61  | B2    | 1808 | G    |
| 61  | B2    | 1813 | U    |
| 61  | B2    | 1814 | G    |
| 61  | B2    | 1815 | C    |
| 61  | B2    | 1816 | C    |
| 61  | B2    | 1817 | C    |
| 61  | B2    | 1821 | G    |
| 61  | B2    | 1822 | U    |
| 61  | B2    | 1823 | A    |
| 61  | B2    | 1824 | C    |
| 61  | B2    | 1825 | A    |
| 61  | B2    | 1826 | C    |
| 61  | B2    | 1827 | A    |
| 61  | B2    | 1828 | C    |
| 61  | B2    | 1829 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 61  | B2    | 1831 | C    |
| 61  | B2    | 1832 | C    |
| 61  | B2    | 1834 | G    |
| 61  | B2    | 1839 | U    |
| 61  | B2    | 1847 | A    |
| 61  | B2    | 1848 | U    |
| 61  | B2    | 1849 | U    |
| 61  | B2    | 1850 | G    |
| 61  | B2    | 1852 | A    |
| 61  | B2    | 1859 | A    |
| 61  | B2    | 1863 | A    |
| 61  | B2    | 1865 | G    |
| 61  | B2    | 1872 | G    |
| 61  | B2    | 1874 | C    |
| 61  | B2    | 1875 | G    |
| 61  | B2    | 1876 | U    |
| 61  | B2    | 1882 | C    |
| 61  | B2    | 1903 | G    |
| 61  | B2    | 1904 | G    |
| 61  | B2    | 1905 | U    |
| 61  | B2    | 1906 | U    |
| 61  | B2    | 1907 | G    |
| 61  | B2    | 1909 | U    |
| 61  | B2    | 1911 | C    |
| 61  | B2    | 1912 | G    |
| 61  | B2    | 1922 | A    |
| 61  | B2    | 1936 | U    |
| 61  | B2    | 1942 | G    |
| 61  | B2    | 1949 | A    |
| 61  | B2    | 1950 | A    |
| 61  | B2    | 1952 | G    |
| 61  | B2    | 1955 | G    |
| 61  | B2    | 1957 | A    |
| 61  | B2    | 1961 | A    |
| 61  | B2    | 1962 | G    |
| 61  | B2    | 1964 | U    |
| 61  | B2    | 1966 | U    |
| 61  | B2    | 1968 | C    |
| 61  | B2    | 1969 | G    |
| 61  | B2    | 1971 | A    |
| 61  | B2    | 1973 | G    |
| 61  | B2    | 1975 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 61  | B2    | 1986 | A    |
| 61  | B2    | 1987 | G    |
| 61  | B2    | 1988 | G    |
| 61  | B2    | 1989 | A    |
| 61  | B2    | 1991 | C    |
| 61  | B2    | 1993 | U    |
| 61  | B2    | 1994 | U    |
| 61  | B2    | 1995 | A    |
| 62  | A5    | 3    | A    |
| 62  | A5    | 4    | U    |
| 62  | A5    | 5    | A    |
| 62  | A5    | 6    | U    |
| 62  | A5    | 10   | A    |
| 62  | A5    | 13   | U    |
| 62  | A5    | 15   | A    |
| 62  | A5    | 18   | U    |
| 62  | A5    | 19   | C    |
| 62  | A5    | 25   | G    |
| 62  | A5    | 26   | G    |
| 62  | A5    | 27   | A    |
| 62  | A5    | 29   | U    |
| 62  | A5    | 30   | A    |
| 62  | A5    | 33   | C    |
| 62  | A5    | 34   | C    |
| 62  | A5    | 35   | C    |
| 62  | A5    | 36   | U    |
| 62  | A5    | 40   | U    |
| 62  | A5    | 44   | A    |
| 62  | A5    | 45   | G    |
| 62  | A5    | 47   | A    |
| 62  | A5    | 49   | A    |
| 62  | A5    | 50   | U    |
| 62  | A5    | 52   | A    |
| 62  | A5    | 53   | A    |
| 62  | A5    | 54   | U    |
| 62  | A5    | 55   | U    |
| 62  | A5    | 56   | A    |
| 62  | A5    | 57   | G    |
| 62  | A5    | 58   | G    |
| 62  | A5    | 59   | G    |
| 62  | A5    | 61   | A    |
| 62  | A5    | 63   | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 62  | A5    | 64  | A    |
| 62  | A5    | 69  | A    |
| 62  | A5    | 70  | A    |
| 62  | A5    | 71  | A    |
| 62  | A5    | 72  | C    |
| 62  | A5    | 74  | A    |
| 62  | A5    | 76  | C    |
| 62  | A5    | 77  | A    |
| 62  | A5    | 78  | A    |
| 62  | A5    | 81  | A    |
| 62  | A5    | 83  | U    |
| 62  | A5    | 88  | U    |
| 62  | A5    | 89  | A    |
| 62  | A5    | 90  | G    |
| 62  | A5    | 91  | U    |
| 62  | A5    | 94  | C    |
| 62  | A5    | 95  | G    |
| 62  | A5    | 96  | G    |
| 62  | A5    | 97  | C    |
| 62  | A5    | 98  | G    |
| 62  | A5    | 100 | G    |
| 62  | A5    | 101 | C    |
| 62  | A5    | 105 | A    |
| 62  | A5    | 112 | C    |
| 62  | A5    | 113 | A    |
| 62  | A5    | 114 | G    |
| 62  | A5    | 116 | U    |
| 62  | A5    | 117 | C    |
| 62  | A5    | 120 | C    |
| 62  | A5    | 121 | A    |
| 62  | A5    | 122 | C    |
| 62  | A5    | 123 | U    |
| 62  | A5    | 124 | A    |
| 62  | A5    | 126 | G    |
| 62  | A5    | 127 | U    |
| 62  | A5    | 136 | C    |
| 62  | A5    | 137 | U    |
| 62  | A5    | 138 | A    |
| 62  | A5    | 139 | U    |
| 62  | A5    | 140 | A    |
| 62  | A5    | 141 | U    |
| 62  | A5    | 142 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 62  | A5    | 143 | G    |
| 62  | A5    | 145 | A    |
| 62  | A5    | 148 | U    |
| 62  | A5    | 149 | G    |
| 62  | A5    | 150 | U    |
| 62  | A5    | 154 | A    |
| 62  | A5    | 155 | U    |
| 62  | A5    | 156 | G    |
| 62  | A5    | 158 | A    |
| 62  | A5    | 161 | G    |
| 62  | A5    | 162 | U    |
| 62  | A5    | 163 | A    |
| 62  | A5    | 164 | U    |
| 62  | A5    | 165 | G    |
| 62  | A5    | 167 | A    |
| 62  | A5    | 172 | C    |
| 62  | A5    | 176 | A    |
| 62  | A5    | 177 | U    |
| 62  | A5    | 185 | U    |
| 62  | A5    | 187 | A    |
| 62  | A5    | 188 | G    |
| 62  | A5    | 189 | A    |
| 62  | A5    | 190 | A    |
| 62  | A5    | 191 | A    |
| 62  | A5    | 194 | A    |
| 62  | A5    | 197 | G    |
| 62  | A5    | 198 | A    |
| 62  | A5    | 201 | U    |
| 62  | A5    | 202 | A    |
| 62  | A5    | 205 | U    |
| 62  | A5    | 211 | U    |
| 62  | A5    | 212 | U    |
| 62  | A5    | 213 | A    |
| 62  | A5    | 214 | A    |
| 62  | A5    | 215 | A    |
| 62  | A5    | 220 | G    |
| 62  | A5    | 222 | C    |
| 62  | A5    | 225 | U    |
| 62  | A5    | 226 | U    |
| 62  | A5    | 228 | C    |
| 62  | A5    | 229 | C    |
| 62  | A5    | 232 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 62  | A5    | 233 | A    |
| 62  | A5    | 234 | G    |
| 62  | A5    | 236 | G    |
| 62  | A5    | 237 | G    |
| 62  | A5    | 239 | U    |
| 62  | A5    | 240 | G    |
| 62  | A5    | 241 | C    |
| 62  | A5    | 242 | C    |
| 62  | A5    | 248 | C    |
| 62  | A5    | 253 | A    |
| 62  | A5    | 259 | A    |
| 62  | A5    | 260 | A    |
| 62  | A5    | 262 | G    |
| 62  | A5    | 263 | A    |
| 62  | A5    | 273 | G    |
| 62  | A5    | 275 | U    |
| 62  | A5    | 279 | U    |
| 62  | A5    | 280 | C    |
| 62  | A5    | 282 | A    |
| 62  | A5    | 284 | A    |
| 62  | A5    | 287 | G    |
| 62  | A5    | 296 | C    |
| 62  | A5    | 301 | U    |
| 62  | A5    | 302 | A    |
| 62  | A5    | 303 | G    |
| 62  | A5    | 307 | A    |
| 62  | A5    | 313 | A    |
| 62  | A5    | 314 | A    |
| 62  | A5    | 316 | U    |
| 62  | A5    | 319 | G    |
| 62  | A5    | 322 | G    |
| 62  | A5    | 323 | U    |
| 62  | A5    | 326 | A    |
| 62  | A5    | 328 | U    |
| 62  | A5    | 329 | C    |
| 62  | A5    | 339 | C    |
| 62  | A5    | 340 | U    |
| 62  | A5    | 341 | A    |
| 62  | A5    | 342 | A    |
| 62  | A5    | 345 | A    |
| 62  | A5    | 347 | A    |
| 62  | A5    | 351 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 62  | A5    | 354 | A    |
| 62  | A5    | 355 | G    |
| 62  | A5    | 356 | A    |
| 62  | A5    | 357 | C    |
| 62  | A5    | 360 | A    |
| 62  | A5    | 361 | U    |
| 62  | A5    | 365 | A    |
| 62  | A5    | 366 | A    |
| 62  | A5    | 367 | A    |
| 62  | A5    | 368 | C    |
| 62  | A5    | 369 | A    |
| 62  | A5    | 370 | A    |
| 62  | A5    | 371 | G    |
| 62  | A5    | 372 | U    |
| 62  | A5    | 375 | C    |
| 62  | A5    | 376 | G    |
| 62  | A5    | 377 | U    |
| 62  | A5    | 378 | G    |
| 62  | A5    | 380 | G    |
| 62  | A5    | 382 | G    |
| 62  | A5    | 384 | A    |
| 62  | A5    | 386 | G    |
| 62  | A5    | 388 | U    |
| 62  | A5    | 389 | G    |
| 62  | A5    | 390 | A    |
| 62  | A5    | 392 | A    |
| 62  | A5    | 393 | A    |
| 62  | A5    | 394 | G    |
| 62  | A5    | 397 | C    |
| 62  | A5    | 403 | A    |
| 62  | A5    | 404 | U    |
| 62  | A5    | 405 | A    |
| 62  | A5    | 407 | A    |
| 62  | A5    | 413 | A    |
| 62  | A5    | 414 | A    |
| 62  | A5    | 416 | C    |
| 62  | A5    | 417 | A    |
| 62  | A5    | 418 | G    |
| 62  | A5    | 419 | U    |
| 62  | A5    | 420 | A    |
| 62  | A5    | 421 | C    |
| 62  | A5    | 428 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 62  | A5    | 429 | U    |
| 62  | A5    | 436 | A    |
| 62  | A5    | 439 | U    |
| 62  | A5    | 440 | U    |
| 62  | A5    | 441 | A    |
| 62  | A5    | 444 | C    |
| 62  | A5    | 448 | A    |
| 62  | A5    | 449 | U    |
| 62  | A5    | 450 | G    |
| 62  | A5    | 453 | C    |
| 62  | A5    | 457 | A    |
| 62  | A5    | 458 | A    |
| 62  | A5    | 459 | U    |
| 62  | A5    | 460 | A    |
| 62  | A5    | 461 | U    |
| 62  | A5    | 462 | C    |
| 62  | A5    | 463 | C    |
| 62  | A5    | 464 | G    |
| 62  | A5    | 465 | U    |
| 62  | A5    | 466 | U    |
| 62  | A5    | 467 | A    |
| 62  | A5    | 471 | A    |
| 62  | A5    | 473 | A    |
| 62  | A5    | 474 | A    |
| 62  | A5    | 475 | U    |
| 62  | A5    | 476 | U    |
| 62  | A5    | 477 | C    |
| 62  | A5    | 479 | U    |
| 62  | A5    | 482 | U    |
| 62  | A5    | 485 | A    |
| 62  | A5    | 486 | A    |
| 62  | A5    | 487 | A    |
| 62  | A5    | 497 | U    |
| 62  | A5    | 507 | U    |
| 62  | A5    | 516 | U    |
| 62  | A5    | 521 | U    |
| 62  | A5    | 522 | G    |
| 62  | A5    | 523 | C    |
| 62  | A5    | 524 | A    |
| 62  | A5    | 525 | U    |
| 62  | A5    | 526 | U    |
| 62  | A5    | 527 | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 62  | A5    | 530 | U    |
| 62  | A5    | 536 | U    |
| 62  | A5    | 537 | A    |
| 62  | A5    | 538 | A    |
| 62  | A5    | 539 | G    |
| 62  | A5    | 540 | G    |
| 62  | A5    | 541 | A    |
| 62  | A5    | 542 | C    |
| 62  | A5    | 543 | A    |
| 62  | A5    | 547 | U    |
| 62  | A5    | 553 | A    |
| 62  | A5    | 554 | U    |
| 62  | A5    | 559 | A    |
| 62  | A5    | 562 | U    |
| 62  | A5    | 565 | C    |
| 62  | A5    | 568 | A    |
| 62  | A5    | 569 | U    |
| 62  | A5    | 576 | U    |
| 62  | A5    | 577 | A    |
| 62  | A5    | 578 | A    |
| 62  | A5    | 580 | A    |
| 62  | A5    | 581 | U    |
| 62  | A5    | 583 | U    |
| 62  | A5    | 584 | A    |
| 62  | A5    | 588 | U    |
| 62  | A5    | 591 | A    |
| 62  | A5    | 593 | U    |
| 62  | A5    | 596 | A    |
| 62  | A5    | 616 | A    |
| 62  | A5    | 620 | U    |
| 62  | A5    | 621 | A    |
| 62  | A5    | 622 | A    |
| 62  | A5    | 623 | C    |
| 62  | A5    | 625 | C    |
| 62  | A5    | 626 | A    |
| 62  | A5    | 632 | A    |
| 62  | A5    | 641 | A    |
| 62  | A5    | 642 | A    |
| 62  | A5    | 643 | U    |
| 62  | A5    | 644 | U    |
| 62  | A5    | 648 | U    |
| 62  | A5    | 652 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 62  | A5    | 653 | U    |
| 62  | A5    | 657 | G    |
| 62  | A5    | 665 | U    |
| 62  | A5    | 666 | A    |
| 62  | A5    | 667 | U    |
| 62  | A5    | 668 | A    |
| 62  | A5    | 669 | U    |
| 62  | A5    | 670 | G    |
| 62  | A5    | 671 | A    |
| 62  | A5    | 672 | U    |
| 62  | A5    | 673 | U    |
| 62  | A5    | 674 | A    |
| 62  | A5    | 676 | A    |
| 62  | A5    | 681 | G    |
| 62  | A5    | 685 | A    |
| 62  | A5    | 690 | U    |
| 62  | A5    | 696 | U    |
| 62  | A5    | 697 | U    |
| 62  | A5    | 698 | A    |
| 62  | A5    | 699 | U    |
| 62  | A5    | 700 | A    |
| 62  | A5    | 701 | U    |
| 62  | A5    | 702 | A    |
| 62  | A5    | 703 | A    |
| 62  | A5    | 704 | U    |
| 62  | A5    | 713 | U    |
| 62  | A5    | 716 | C    |
| 62  | A5    | 718 | U    |
| 62  | A5    | 719 | U    |
| 62  | A5    | 720 | G    |
| 62  | A5    | 723 | U    |
| 62  | A5    | 726 | U    |
| 62  | A5    | 733 | A    |
| 62  | A5    | 739 | U    |
| 62  | A5    | 740 | G    |
| 62  | A5    | 743 | C    |
| 62  | A5    | 745 | U    |
| 62  | A5    | 746 | G    |
| 62  | A5    | 747 | U    |
| 62  | A5    | 748 | A    |
| 62  | A5    | 749 | U    |
| 62  | A5    | 750 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 62  | A5    | 751 | A    |
| 62  | A5    | 752 | U    |
| 62  | A5    | 753 | U    |
| 62  | A5    | 754 | A    |
| 62  | A5    | 756 | C    |
| 62  | A5    | 760 | G    |
| 62  | A5    | 761 | C    |
| 62  | A5    | 762 | G    |
| 62  | A5    | 763 | A    |
| 62  | A5    | 765 | A    |
| 62  | A5    | 766 | G    |
| 62  | A5    | 768 | U    |
| 62  | A5    | 771 | A    |
| 62  | A5    | 772 | G    |
| 62  | A5    | 774 | A    |
| 62  | A5    | 775 | U    |
| 62  | A5    | 776 | A    |
| 62  | A5    | 783 | G    |
| 62  | A5    | 786 | C    |
| 62  | A5    | 787 | C    |
| 62  | A5    | 791 | C    |
| 62  | A5    | 792 | U    |
| 62  | A5    | 795 | A    |
| 62  | A5    | 797 | A    |
| 62  | A5    | 798 | C    |
| 62  | A5    | 799 | A    |
| 62  | A5    | 800 | C    |
| 62  | A5    | 801 | G    |
| 62  | A5    | 803 | A    |
| 62  | A5    | 804 | C    |
| 62  | A5    | 805 | C    |
| 62  | A5    | 811 | G    |
| 62  | A5    | 816 | A    |
| 62  | A5    | 821 | U    |
| 62  | A5    | 823 | U    |
| 62  | A5    | 827 | A    |
| 62  | A5    | 830 | U    |
| 62  | A5    | 831 | A    |
| 62  | A5    | 832 | U    |
| 62  | A5    | 833 | U    |
| 62  | A5    | 834 | G    |
| 62  | A5    | 835 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 62  | A5    | 838 | U    |
| 62  | A5    | 839 | A    |
| 62  | A5    | 840 | U    |
| 62  | A5    | 841 | A    |
| 62  | A5    | 842 | A    |
| 62  | A5    | 849 | U    |
| 62  | A5    | 851 | G    |
| 62  | A5    | 852 | C    |
| 62  | A5    | 855 | A    |
| 62  | A5    | 856 | A    |
| 62  | A5    | 858 | U    |
| 62  | A5    | 859 | A    |
| 62  | A5    | 860 | A    |
| 62  | A5    | 862 | U    |
| 62  | A5    | 865 | A    |
| 62  | A5    | 866 | C    |
| 62  | A5    | 867 | U    |
| 62  | A5    | 869 | A    |
| 62  | A5    | 870 | U    |
| 62  | A5    | 871 | A    |
| 62  | A5    | 872 | A    |
| 62  | A5    | 873 | U    |
| 62  | A5    | 874 | G    |
| 62  | A5    | 879 | U    |
| 62  | A5    | 894 | U    |
| 62  | A5    | 895 | U    |
| 62  | A5    | 897 | U    |
| 62  | A5    | 898 | A    |
| 62  | A5    | 899 | G    |
| 62  | A5    | 902 | A    |
| 62  | A5    | 905 | U    |
| 62  | A5    | 907 | A    |
| 62  | A5    | 909 | A    |
| 62  | A5    | 913 | U    |
| 62  | A5    | 914 | C    |
| 62  | A5    | 917 | G    |
| 62  | A5    | 925 | C    |
| 62  | A5    | 928 | U    |
| 62  | A5    | 929 | A    |
| 62  | A5    | 930 | U    |
| 62  | A5    | 931 | A    |
| 62  | A5    | 964 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 62  | A5    | 966  | U    |
| 62  | A5    | 967  | C    |
| 62  | A5    | 968  | U    |
| 62  | A5    | 969  | A    |
| 62  | A5    | 974  | G    |
| 62  | A5    | 978  | G    |
| 62  | A5    | 979  | U    |
| 62  | A5    | 980  | A    |
| 62  | A5    | 981  | C    |
| 62  | A5    | 982  | C    |
| 62  | A5    | 983  | U    |
| 62  | A5    | 984  | U    |
| 62  | A5    | 986  | A    |
| 62  | A5    | 990  | U    |
| 62  | A5    | 1000 | G    |
| 62  | A5    | 1001 | A    |
| 62  | A5    | 1003 | C    |
| 62  | A5    | 1004 | C    |
| 62  | A5    | 1006 | A    |
| 62  | A5    | 1007 | A    |
| 62  | A5    | 1008 | A    |
| 62  | A5    | 1009 | G    |
| 62  | A5    | 1012 | G    |
| 62  | A5    | 1013 | G    |
| 62  | A5    | 1014 | U    |
| 62  | A5    | 1015 | G    |
| 62  | A5    | 1017 | A    |
| 62  | A5    | 1018 | C    |
| 62  | A5    | 1019 | U    |
| 62  | A5    | 1022 | A    |
| 62  | A5    | 1026 | G    |
| 62  | A5    | 1030 | A    |
| 62  | A5    | 1031 | G    |
| 62  | A5    | 1032 | G    |
| 62  | A5    | 1033 | U    |
| 62  | A5    | 1034 | U    |
| 62  | A5    | 1035 | G    |
| 62  | A5    | 1041 | A    |
| 62  | A5    | 1046 | A    |
| 62  | A5    | 1047 | A    |
| 62  | A5    | 1049 | C    |
| 62  | A5    | 1050 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 62  | A5    | 1052 | U    |
| 62  | A5    | 1054 | A    |
| 62  | A5    | 1056 | G    |
| 62  | A5    | 1059 | A    |
| 62  | A5    | 1060 | G    |
| 62  | A5    | 1065 | A    |
| 62  | A5    | 1066 | A    |
| 62  | A5    | 1067 | A    |
| 62  | A5    | 1068 | C    |
| 62  | A5    | 1069 | A    |
| 62  | A5    | 1070 | G    |
| 62  | A5    | 1071 | U    |
| 62  | A5    | 1072 | U    |
| 62  | A5    | 1074 | U    |
| 62  | A5    | 1077 | C    |
| 62  | A5    | 1079 | U    |
| 62  | A5    | 1080 | G    |
| 62  | A5    | 1081 | C    |
| 62  | A5    | 1082 | A    |
| 62  | A5    | 1084 | A    |
| 62  | A5    | 1087 | G    |
| 62  | A5    | 1092 | U    |
| 62  | A5    | 1094 | A    |
| 62  | A5    | 1095 | G    |
| 62  | A5    | 1096 | A    |
| 62  | A5    | 1097 | A    |
| 62  | A5    | 1106 | A    |
| 62  | A5    | 1107 | G    |
| 62  | A5    | 1108 | G    |
| 62  | A5    | 1109 | G    |
| 62  | A5    | 1112 | G    |
| 62  | A5    | 1113 | A    |
| 62  | A5    | 1114 | A    |
| 62  | A5    | 1115 | A    |
| 62  | A5    | 1116 | G    |
| 62  | A5    | 1117 | A    |
| 62  | A5    | 1120 | A    |
| 62  | A5    | 1121 | A    |
| 62  | A5    | 1122 | U    |
| 62  | A5    | 1123 | C    |
| 62  | A5    | 1124 | G    |
| 62  | A5    | 1125 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 62  | A5    | 1126 | A    |
| 62  | A5    | 1129 | A    |
| 62  | A5    | 1132 | U    |
| 62  | A5    | 1133 | A    |
| 62  | A5    | 1137 | G    |
| 62  | A5    | 1141 | G    |
| 62  | A5    | 1143 | U    |
| 62  | A5    | 1144 | C    |
| 62  | A5    | 1151 | A    |
| 62  | A5    | 1153 | G    |
| 62  | A5    | 1156 | U    |
| 62  | A5    | 1158 | C    |
| 62  | A5    | 1159 | C    |
| 62  | A5    | 1160 | U    |
| 62  | A5    | 1161 | C    |
| 62  | A5    | 1162 | A    |
| 62  | A5    | 1163 | G    |
| 62  | A5    | 1164 | G    |
| 62  | A5    | 1165 | A    |
| 62  | A5    | 1174 | G    |
| 62  | A5    | 1176 | A    |
| 62  | A5    | 1178 | U    |
| 62  | A5    | 1179 | U    |
| 62  | A5    | 1180 | U    |
| 62  | A5    | 1181 | A    |
| 62  | A5    | 1182 | A    |
| 62  | A5    | 1183 | U    |
| 62  | A5    | 1193 | A    |
| 62  | A5    | 1194 | A    |
| 62  | A5    | 1195 | U    |
| 62  | A5    | 1196 | A    |
| 62  | A5    | 1197 | A    |
| 62  | A5    | 1198 | U    |
| 62  | A5    | 1205 | U    |
| 62  | A5    | 1206 | G    |
| 62  | A5    | 1207 | G    |
| 62  | A5    | 1208 | U    |
| 62  | A5    | 1211 | A    |
| 62  | A5    | 1213 | C    |
| 62  | A5    | 1215 | A    |
| 62  | A5    | 1223 | G    |
| 62  | A5    | 1226 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 62  | A5    | 1227 | C    |
| 62  | A5    | 1228 | C    |
| 62  | A5    | 1229 | U    |
| 62  | A5    | 1230 | U    |
| 62  | A5    | 1231 | A    |
| 62  | A5    | 1232 | G    |
| 62  | A5    | 1233 | G    |
| 62  | A5    | 1234 | G    |
| 62  | A5    | 1240 | A    |
| 62  | A5    | 1242 | G    |
| 62  | A5    | 1245 | C    |
| 62  | A5    | 1249 | A    |
| 62  | A5    | 1254 | U    |
| 62  | A5    | 1260 | A    |
| 62  | A5    | 1262 | C    |
| 62  | A5    | 1263 | U    |
| 62  | A5    | 1265 | U    |
| 62  | A5    | 1271 | G    |
| 62  | A5    | 1272 | G    |
| 62  | A5    | 1276 | G    |
| 62  | A5    | 1277 | A    |
| 62  | A5    | 1278 | A    |
| 62  | A5    | 1279 | C    |
| 62  | A5    | 1281 | U    |
| 62  | A5    | 1284 | A    |
| 62  | A5    | 1287 | U    |
| 62  | A5    | 1288 | U    |
| 62  | A5    | 1291 | U    |
| 62  | A5    | 1293 | A    |
| 62  | A5    | 1294 | U    |
| 62  | A5    | 1295 | A    |
| 62  | A5    | 1296 | U    |
| 62  | A5    | 1297 | G    |
| 62  | A5    | 1298 | A    |
| 62  | A5    | 1301 | A    |
| 62  | A5    | 1307 | G    |
| 62  | A5    | 1308 | U    |
| 62  | A5    | 1309 | U    |
| 62  | A5    | 1310 | A    |
| 62  | A5    | 1311 | U    |
| 62  | A5    | 1315 | A    |
| 62  | A5    | 1316 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 62  | A5    | 1317 | A    |
| 62  | A5    | 1321 | G    |
| 62  | A5    | 1323 | C    |
| 62  | A5    | 1324 | C    |
| 62  | A5    | 1329 | G    |
| 62  | A5    | 1330 | G    |
| 62  | A5    | 1331 | G    |
| 62  | A5    | 1332 | C    |
| 62  | A5    | 1339 | U    |
| 62  | A5    | 1342 | U    |
| 62  | A5    | 1343 | A    |
| 62  | A5    | 1347 | A    |
| 62  | A5    | 1349 | A    |
| 62  | A5    | 1350 | A    |
| 62  | A5    | 1352 | U    |
| 62  | A5    | 1353 | G    |
| 62  | A5    | 1357 | C    |
| 62  | A5    | 1358 | U    |
| 62  | A5    | 1360 | U    |
| 62  | A5    | 1361 | G    |
| 62  | A5    | 1362 | G    |
| 62  | A5    | 1365 | U    |
| 62  | A5    | 1366 | G    |
| 62  | A5    | 1368 | A    |
| 62  | A5    | 1369 | C    |
| 62  | A5    | 1373 | A    |
| 62  | A5    | 1374 | C    |
| 62  | A5    | 1375 | G    |
| 62  | A5    | 1376 | U    |
| 62  | A5    | 1378 | A    |
| 62  | A5    | 1379 | U    |
| 62  | A5    | 1382 | U    |
| 62  | A5    | 1383 | A    |
| 62  | A5    | 1384 | C    |
| 62  | A5    | 1385 | G    |
| 62  | A5    | 1386 | U    |
| 62  | A5    | 1387 | G    |
| 62  | A5    | 1389 | C    |
| 62  | A5    | 1390 | C    |
| 62  | A5    | 1391 | A    |
| 62  | A5    | 1393 | A    |
| 62  | A5    | 1394 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 62  | A5    | 1395 | U    |
| 62  | A5    | 1396 | A    |
| 62  | A5    | 1397 | A    |
| 62  | A5    | 1400 | A    |
| 62  | A5    | 1403 | C    |
| 62  | A5    | 1405 | U    |
| 62  | A5    | 1407 | C    |
| 62  | A5    | 1411 | U    |
| 62  | A5    | 1412 | A    |
| 62  | A5    | 1413 | C    |
| 62  | A5    | 1414 | C    |
| 62  | A5    | 1418 | A    |
| 62  | A5    | 1423 | C    |
| 62  | A5    | 1424 | G    |
| 62  | A5    | 1428 | G    |
| 62  | A5    | 1430 | U    |
| 62  | A5    | 1432 | C    |
| 62  | A5    | 1435 | A    |
| 62  | A5    | 1436 | A    |
| 62  | A5    | 1437 | A    |
| 62  | A5    | 1438 | A    |
| 62  | A5    | 1442 | C    |
| 62  | A5    | 1443 | A    |
| 62  | A5    | 1447 | C    |
| 62  | A5    | 1449 | G    |
| 62  | A5    | 1451 | G    |
| 62  | A5    | 1452 | A    |
| 62  | A5    | 1453 | U    |
| 62  | A5    | 1454 | C    |
| 62  | A5    | 1456 | U    |
| 62  | A5    | 1458 | G    |
| 62  | A5    | 1459 | A    |
| 62  | A5    | 1460 | A    |
| 62  | A5    | 1461 | G    |
| 62  | A5    | 1463 | C    |
| 62  | A5    | 1464 | G    |
| 62  | A5    | 1465 | A    |
| 62  | A5    | 1468 | U    |
| 62  | A5    | 1470 | C    |
| 62  | A5    | 1473 | U    |
| 62  | A5    | 1477 | G    |
| 62  | A5    | 1478 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 62  | A5    | 1480 | U    |
| 62  | A5    | 1481 | G    |
| 62  | A5    | 1483 | G    |
| 62  | A5    | 1484 | U    |
| 62  | A5    | 1485 | A    |
| 62  | A5    | 1486 | A    |
| 62  | A5    | 1488 | A    |
| 62  | A5    | 1492 | C    |
| 62  | A5    | 1500 | G    |
| 62  | A5    | 1501 | A    |
| 62  | A5    | 1502 | A    |
| 62  | A5    | 1506 | A    |
| 62  | A5    | 1507 | C    |
| 62  | A5    | 1510 | G    |
| 62  | A5    | 1511 | C    |
| 62  | A5    | 1512 | C    |
| 62  | A5    | 1513 | C    |
| 62  | A5    | 1515 | U    |
| 62  | A5    | 1516 | A    |
| 62  | A5    | 1517 | A    |
| 62  | A5    | 1519 | A    |
| 62  | A5    | 1520 | U    |
| 62  | A5    | 1521 | G    |
| 62  | A5    | 1522 | G    |
| 62  | A5    | 1523 | A    |
| 62  | A5    | 1524 | U    |
| 62  | A5    | 1528 | G    |
| 62  | A5    | 1529 | C    |
| 62  | A5    | 1531 | U    |
| 62  | A5    | 1532 | A    |
| 62  | A5    | 1533 | A    |
| 62  | A5    | 1539 | A    |
| 62  | A5    | 1540 | U    |
| 62  | A5    | 1542 | C    |
| 62  | A5    | 1544 | U    |
| 62  | A5    | 1545 | A    |
| 62  | A5    | 1546 | U    |
| 62  | A5    | 1547 | A    |
| 62  | A5    | 1548 | C    |
| 62  | A5    | 1552 | A    |
| 62  | A5    | 1564 | G    |
| 62  | A5    | 1565 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 62  | A5    | 1566 | U    |
| 62  | A5    | 1567 | G    |
| 62  | A5    | 1570 | U    |
| 62  | A5    | 1572 | A    |
| 62  | A5    | 1574 | A    |
| 62  | A5    | 1575 | U    |
| 62  | A5    | 1576 | U    |
| 62  | A5    | 1577 | A    |
| 62  | A5    | 1578 | C    |
| 62  | A5    | 1580 | U    |
| 62  | A5    | 1581 | G    |
| 62  | A5    | 1583 | G    |
| 62  | A5    | 1584 | A    |
| 62  | A5    | 1592 | U    |
| 62  | A5    | 1593 | U    |
| 62  | A5    | 1595 | G    |
| 62  | A5    | 1596 | A    |
| 62  | A5    | 1598 | A    |
| 62  | A5    | 1603 | A    |
| 62  | A5    | 1605 | U    |
| 62  | A5    | 1606 | G    |
| 62  | A5    | 1607 | A    |
| 62  | A5    | 1609 | U    |
| 62  | A5    | 1610 | A    |
| 62  | A5    | 1611 | G    |
| 62  | A5    | 1613 | A    |
| 62  | A5    | 1615 | G    |
| 62  | A5    | 1617 | U    |
| 62  | A5    | 1623 | G    |
| 62  | A5    | 1627 | U    |
| 62  | A5    | 1628 | G    |
| 62  | A5    | 1629 | C    |
| 62  | A5    | 1631 | U    |
| 62  | A5    | 1633 | G    |
| 62  | A5    | 1634 | A    |
| 62  | A5    | 1635 | A    |
| 62  | A5    | 1640 | U    |
| 62  | A5    | 1641 | U    |
| 62  | A5    | 1646 | U    |
| 62  | A5    | 1650 | C    |
| 62  | A5    | 1661 | C    |
| 62  | A5    | 1662 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 62  | A5    | 1667 | U    |
| 62  | A5    | 1668 | U    |
| 62  | A5    | 1669 | G    |
| 62  | A5    | 1672 | A    |
| 62  | A5    | 1673 | C    |
| 62  | A5    | 1675 | G    |
| 62  | A5    | 1676 | A    |
| 62  | A5    | 1678 | C    |
| 62  | A5    | 1682 | G    |
| 62  | A5    | 1684 | G    |
| 62  | A5    | 1687 | U    |
| 62  | A5    | 1688 | A    |
| 62  | A5    | 1689 | G    |
| 62  | A5    | 1690 | U    |
| 62  | A5    | 1691 | A    |
| 62  | A5    | 1692 | G    |
| 62  | A5    | 1694 | A    |
| 62  | A5    | 1695 | A    |
| 62  | A5    | 1697 | U    |
| 62  | A5    | 1698 | A    |
| 62  | A5    | 1701 | C    |
| 62  | A5    | 1702 | G    |
| 62  | A5    | 1705 | U    |
| 62  | A5    | 1707 | A    |
| 62  | A5    | 1708 | G    |
| 62  | A5    | 1711 | C    |
| 62  | A5    | 1712 | C    |
| 62  | A5    | 1713 | U    |
| 62  | A5    | 1715 | G    |
| 62  | A5    | 1716 | G    |
| 62  | A5    | 1717 | A    |
| 62  | A5    | 1718 | G    |
| 62  | A5    | 1719 | G    |
| 62  | A5    | 1720 | A    |
| 62  | A5    | 1723 | G    |
| 62  | A5    | 1724 | A    |
| 62  | A5    | 1725 | A    |
| 62  | A5    | 1726 | G    |
| 62  | A5    | 1727 | U    |
| 62  | A5    | 1732 | A    |
| 62  | A5    | 1733 | A    |
| 62  | A5    | 1734 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 62  | A5    | 1735 | G    |
| 62  | A5    | 1736 | G    |
| 62  | A5    | 1744 | U    |
| 62  | A5    | 1745 | G    |
| 62  | A5    | 1746 | A    |
| 62  | A5    | 1747 | A    |
| 62  | A5    | 1748 | C    |
| 62  | A5    | 1750 | G    |
| 62  | A5    | 1751 | U    |
| 62  | A5    | 1753 | G    |
| 62  | A5    | 1755 | U    |
| 62  | A5    | 1756 | G    |
| 62  | A5    | 1757 | A    |
| 62  | A5    | 1759 | C    |
| 62  | A5    | 1763 | A    |
| 62  | A5    | 1765 | U    |
| 62  | A5    | 1766 | U    |
| 62  | A5    | 1769 | U    |
| 62  | A5    | 1773 | U    |
| 62  | A5    | 1774 | C    |
| 62  | A5    | 1778 | A    |
| 62  | A5    | 1779 | G    |
| 62  | A5    | 1780 | U    |
| 62  | A5    | 1781 | U    |
| 62  | A5    | 1782 | C    |
| 62  | A5    | 1783 | A    |
| 62  | A5    | 1785 | G    |
| 62  | A5    | 1786 | G    |
| 62  | A5    | 1787 | C    |
| 62  | A5    | 1790 | A    |
| 62  | A5    | 1791 | A    |
| 62  | A5    | 1794 | G    |
| 62  | A5    | 1795 | A    |
| 62  | A5    | 1796 | A    |
| 62  | A5    | 1797 | A    |
| 62  | A5    | 1798 | A    |
| 62  | A5    | 1799 | U    |
| 62  | A5    | 1801 | U    |
| 62  | A5    | 1802 | U    |
| 62  | A5    | 1803 | C    |
| 62  | A5    | 1804 | A    |
| 62  | A5    | 1805 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 62  | A5    | 1806 | G    |
| 62  | A5    | 1809 | A    |
| 62  | A5    | 1810 | A    |
| 62  | A5    | 1813 | A    |
| 62  | A5    | 1861 | A    |
| 62  | A5    | 1863 | U    |
| 62  | A5    | 1864 | U    |
| 62  | A5    | 1865 | U    |
| 62  | A5    | 1867 | A    |
| 62  | A5    | 1868 | A    |
| 62  | A5    | 1869 | C    |
| 62  | A5    | 1871 | A    |
| 62  | A5    | 1872 | A    |
| 62  | A5    | 1873 | A    |
| 62  | A5    | 1874 | G    |
| 62  | A5    | 1876 | G    |
| 62  | A5    | 1877 | A    |
| 62  | A5    | 1879 | U    |
| 62  | A5    | 1880 | A    |
| 62  | A5    | 1883 | G    |
| 62  | A5    | 1888 | A    |
| 62  | A5    | 1889 | A    |
| 62  | A5    | 1890 | U    |
| 62  | A5    | 1892 | C    |
| 62  | A5    | 1893 | C    |
| 62  | A5    | 1899 | C    |
| 62  | A5    | 1907 | U    |
| 62  | A5    | 1908 | A    |
| 62  | A5    | 1909 | U    |
| 62  | A5    | 1910 | C    |
| 62  | A5    | 1911 | C    |
| 62  | A5    | 1913 | U    |
| 62  | A5    | 1914 | U    |
| 62  | A5    | 1921 | U    |
| 62  | A5    | 1923 | A    |
| 62  | A5    | 1925 | U    |
| 62  | A5    | 1926 | A    |
| 62  | A5    | 1927 | U    |
| 62  | A5    | 1934 | C    |
| 62  | A5    | 1935 | G    |
| 62  | A5    | 1936 | U    |
| 62  | A5    | 1937 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 62  | A5    | 1941 | A    |
| 62  | A5    | 1942 | U    |
| 62  | A5    | 1943 | C    |
| 62  | A5    | 1946 | G    |
| 62  | A5    | 1954 | G    |
| 62  | A5    | 1955 | A    |
| 62  | A5    | 1956 | A    |
| 62  | A5    | 1957 | C    |
| 62  | A5    | 1958 | G    |
| 62  | A5    | 1959 | A    |
| 62  | A5    | 1961 | C    |
| 62  | A5    | 1963 | U    |
| 62  | A5    | 1965 | A    |
| 62  | A5    | 1968 | A    |
| 62  | A5    | 1969 | A    |
| 62  | A5    | 1970 | G    |
| 62  | A5    | 1971 | C    |
| 62  | A5    | 1972 | C    |
| 62  | A5    | 1973 | G    |
| 62  | A5    | 1974 | U    |
| 62  | A5    | 1975 | C    |
| 62  | A5    | 1988 | A    |
| 62  | A5    | 1994 | U    |
| 62  | A5    | 1995 | U    |
| 62  | A5    | 1999 | U    |
| 62  | A5    | 2000 | U    |
| 62  | A5    | 2001 | U    |
| 62  | A5    | 2002 | C    |
| 62  | A5    | 2003 | U    |
| 62  | A5    | 2005 | U    |
| 62  | A5    | 2006 | U    |
| 62  | A5    | 2008 | U    |
| 62  | A5    | 2010 | U    |
| 62  | A5    | 2011 | A    |
| 62  | A5    | 2014 | C    |
| 62  | A5    | 2015 | G    |
| 62  | A5    | 2016 | U    |
| 62  | A5    | 2017 | A    |
| 62  | A5    | 2026 | G    |
| 62  | A5    | 2028 | A    |
| 62  | A5    | 2029 | G    |
| 62  | A5    | 2030 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 62  | A5    | 2033 | U    |
| 62  | A5    | 2034 | U    |
| 62  | A5    | 2035 | C    |
| 62  | A5    | 2036 | G    |
| 62  | A5    | 2037 | C    |
| 62  | A5    | 2038 | A    |
| 62  | A5    | 2043 | G    |
| 62  | A5    | 2047 | U    |
| 62  | A5    | 2054 | U    |
| 62  | A5    | 2055 | G    |
| 62  | A5    | 2060 | A    |
| 62  | A5    | 2061 | G    |
| 62  | A5    | 2062 | A    |
| 62  | A5    | 2063 | A    |
| 62  | A5    | 2064 | G    |
| 62  | A5    | 2065 | A    |
| 62  | A5    | 2066 | G    |
| 62  | A5    | 2070 | G    |
| 62  | A5    | 2071 | A    |
| 62  | A5    | 2072 | C    |
| 62  | A5    | 2075 | A    |
| 62  | A5    | 2076 | U    |
| 62  | A5    | 2078 | C    |
| 62  | A5    | 2079 | U    |
| 62  | A5    | 2082 | U    |
| 62  | A5    | 2086 | U    |
| 62  | A5    | 2089 | A    |
| 62  | A5    | 2093 | U    |
| 62  | A5    | 2094 | U    |
| 62  | A5    | 2095 | U    |
| 62  | A5    | 2098 | C    |
| 62  | A5    | 2101 | C    |
| 62  | A5    | 2102 | G    |
| 62  | A5    | 2106 | C    |
| 62  | A5    | 2107 | U    |
| 62  | A5    | 2108 | U    |
| 62  | A5    | 2110 | A    |
| 62  | A5    | 2111 | A    |
| 62  | A5    | 2112 | A    |
| 62  | A5    | 2113 | A    |
| 62  | A5    | 2121 | U    |
| 62  | A5    | 2125 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 62  | A5    | 2126 | A    |
| 62  | A5    | 2127 | C    |
| 62  | A5    | 2128 | A    |
| 62  | A5    | 2129 | C    |
| 62  | A5    | 2130 | G    |
| 62  | A5    | 2131 | C    |
| 62  | A5    | 2132 | A    |
| 62  | A5    | 2135 | C    |
| 62  | A5    | 2136 | U    |
| 62  | A5    | 2137 | U    |
| 62  | A5    | 2142 | A    |
| 62  | A5    | 2144 | A    |
| 62  | A5    | 2148 | C    |
| 62  | A5    | 2150 | U    |
| 62  | A5    | 2155 | A    |
| 62  | A5    | 2156 | U    |
| 62  | A5    | 2158 | U    |
| 62  | A5    | 2161 | G    |
| 62  | A5    | 2162 | C    |
| 62  | A5    | 2163 | A    |
| 62  | A5    | 2164 | G    |
| 62  | A5    | 2165 | C    |
| 62  | A5    | 2166 | U    |
| 62  | A5    | 2167 | G    |
| 62  | A5    | 2171 | U    |
| 62  | A5    | 2173 | C    |
| 62  | A5    | 2180 | A    |
| 62  | A5    | 2182 | G    |
| 62  | A5    | 2183 | A    |
| 62  | A5    | 2187 | U    |
| 62  | A5    | 2193 | C    |
| 62  | A5    | 2194 | G    |
| 62  | A5    | 2195 | A    |
| 62  | A5    | 2196 | U    |
| 62  | A5    | 2199 | A    |
| 62  | A5    | 2201 | U    |
| 62  | A5    | 2202 | A    |
| 62  | A5    | 2207 | A    |
| 62  | A5    | 2208 | G    |
| 62  | A5    | 2209 | G    |
| 62  | A5    | 2210 | U    |
| 62  | A5    | 2212 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 62  | A5    | 2213 | G    |
| 62  | A5    | 2214 | G    |
| 62  | A5    | 2215 | G    |
| 62  | A5    | 2216 | A    |
| 62  | A5    | 2217 | A    |
| 62  | A5    | 2218 | G    |
| 62  | A5    | 2219 | U    |
| 62  | A5    | 2220 | C    |
| 62  | A5    | 2222 | G    |
| 62  | A5    | 2224 | A    |
| 62  | A5    | 2229 | A    |
| 62  | A5    | 2234 | C    |
| 62  | A5    | 2236 | U    |
| 62  | A5    | 2239 | C    |
| 62  | A5    | 2240 | U    |
| 62  | A5    | 2244 | G    |
| 62  | A5    | 2246 | A    |
| 62  | A5    | 2249 | A    |
| 62  | A5    | 2251 | G    |
| 62  | A5    | 2255 | G    |
| 62  | A5    | 2268 | G    |
| 62  | A5    | 2269 | A    |
| 62  | A5    | 2270 | G    |
| 62  | A5    | 2467 | A    |
| 62  | A5    | 2468 | A    |
| 62  | A5    | 2469 | U    |
| 62  | A5    | 2470 | U    |
| 62  | A5    | 2471 | A    |
| 62  | A5    | 2472 | A    |
| 62  | A5    | 2473 | C    |
| 62  | A5    | 2477 | C    |
| 62  | A5    | 2479 | A    |
| 62  | A5    | 2480 | U    |
| 62  | A5    | 2481 | U    |
| 62  | A5    | 2482 | C    |
| 62  | A5    | 2486 | A    |
| 62  | A5    | 2490 | G    |
| 62  | A5    | 2491 | C    |
| 62  | A5    | 2494 | G    |
| 62  | A5    | 2495 | G    |
| 62  | A5    | 2496 | A    |
| 62  | A5    | 2497 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 62  | A5    | 2500 | G    |
| 62  | A5    | 2501 | G    |
| 62  | A5    | 2504 | A    |
| 62  | A5    | 2505 | A    |
| 62  | A5    | 2508 | C    |
| 62  | A5    | 2509 | G    |
| 62  | A5    | 2510 | A    |
| 62  | A5    | 2511 | C    |
| 62  | A5    | 2515 | C    |
| 62  | A5    | 2516 | U    |
| 62  | A5    | 2517 | A    |
| 62  | A5    | 2518 | A    |
| 62  | A5    | 2519 | U    |
| 62  | A5    | 2521 | A    |
| 62  | A5    | 2522 | A    |
| 62  | A5    | 2524 | A    |
| 62  | A5    | 2527 | A    |
| 62  | A5    | 2531 | A    |
| 62  | A5    | 2532 | U    |
| 62  | A5    | 2534 | G    |
| 62  | A5    | 2536 | G    |
| 62  | A5    | 2537 | A    |
| 62  | A5    | 2539 | G    |
| 62  | A5    | 2545 | A    |
| 62  | A5    | 2546 | G    |
| 62  | A5    | 2547 | C    |
| 62  | A5    | 2548 | G    |
| 62  | A5    | 2549 | G    |
| 62  | A5    | 2550 | G    |
| 62  | A5    | 2552 | G    |
| 62  | A5    | 2553 | U    |
| 62  | A5    | 2554 | U    |
| 62  | A5    | 2556 | A    |
| 62  | A5    | 2558 | A    |
| 62  | A5    | 2562 | U    |
| 62  | A5    | 2564 | U    |
| 62  | A5    | 2566 | A    |
| 62  | A5    | 2572 | G    |
| 62  | A5    | 2579 | G    |
| 62  | A5    | 2580 | C    |
| 62  | A5    | 2583 | U    |
| 62  | A5    | 2586 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 62  | A5    | 2587 | U    |
| 62  | A5    | 2588 | G    |
| 62  | A5    | 2590 | C    |
| 62  | A5    | 2591 | A    |
| 62  | A5    | 2601 | A    |
| 62  | A5    | 2603 | U    |
| 62  | A5    | 2605 | C    |
| 62  | A5    | 2608 | G    |
| 62  | A5    | 2617 | G    |
| 62  | A5    | 2622 | A    |
| 62  | A5    | 2624 | G    |
| 62  | A5    | 2627 | G    |
| 62  | A5    | 2628 | G    |
| 62  | A5    | 2630 | A    |
| 62  | A5    | 2633 | A    |
| 62  | A5    | 2634 | A    |
| 62  | A5    | 2635 | C    |
| 62  | A5    | 2639 | G    |
| 62  | A5    | 2641 | C    |
| 62  | A5    | 2650 | G    |
| 62  | A5    | 2651 | G    |
| 62  | A5    | 2652 | U    |
| 62  | A5    | 2655 | C    |
| 62  | A5    | 2656 | C    |
| 62  | A5    | 2657 | A    |
| 62  | A5    | 2658 | A    |
| 62  | A5    | 2659 | A    |
| 62  | A5    | 2661 | G    |
| 62  | A5    | 2673 | A    |
| 62  | A5    | 2674 | A    |
| 62  | A5    | 2677 | A    |
| 62  | A5    | 2680 | G    |
| 62  | A5    | 2681 | A    |
| 62  | A5    | 2683 | G    |
| 62  | A5    | 2684 | C    |
| 62  | A5    | 2685 | G    |
| 62  | A5    | 2686 | C    |
| 62  | A5    | 2687 | A    |
| 62  | A5    | 2688 | U    |
| 62  | A5    | 2690 | A    |
| 62  | A5    | 2691 | A    |
| 62  | A5    | 2692 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 62  | A5    | 2693 | G    |
| 62  | A5    | 2697 | U    |
| 62  | A5    | 2698 | A    |
| 62  | A5    | 2701 | G    |
| 62  | A5    | 2702 | A    |
| 62  | A5    | 2703 | G    |
| 62  | A5    | 2706 | U    |
| 62  | A5    | 2707 | C    |
| 62  | A5    | 2711 | C    |
| 62  | A5    | 2713 | G    |
| 62  | A5    | 2714 | U    |
| 62  | A5    | 2715 | C    |
| 62  | A5    | 2717 | C    |
| 62  | A5    | 2720 | U    |
| 62  | A5    | 2725 | U    |
| 62  | A5    | 2726 | A    |
| 62  | A5    | 2727 | U    |
| 62  | A5    | 2732 | C    |
| 62  | A5    | 2735 | A    |
| 62  | A5    | 2737 | C    |
| 62  | A5    | 2742 | G    |
| 62  | A5    | 2743 | C    |
| 62  | A5    | 2744 | C    |
| 62  | A5    | 2749 | G    |
| 62  | A5    | 2750 | A    |
| 62  | A5    | 2751 | A    |
| 62  | A5    | 2752 | C    |
| 62  | A5    | 2753 | G    |
| 62  | A5    | 2754 | G    |
| 62  | A5    | 2756 | C    |
| 62  | A5    | 2757 | U    |
| 62  | A5    | 2761 | A    |
| 62  | A5    | 2763 | U    |
| 62  | A5    | 2766 | U    |
| 62  | A5    | 2767 | U    |
| 62  | A5    | 2769 | G    |
| 62  | A5    | 2770 | C    |
| 62  | A5    | 2771 | G    |
| 62  | A5    | 2772 | G    |
| 62  | A5    | 2775 | A    |
| 62  | A5    | 2776 | A    |
| 62  | A5    | 2777 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 62  | A5    | 2779 | A    |
| 62  | A5    | 2780 | A    |
| 62  | A5    | 2781 | G    |
| 62  | A5    | 2782 | A    |
| 62  | A5    | 2783 | C    |
| 62  | A5    | 2784 | C    |
| 62  | A5    | 2787 | U    |
| 62  | A5    | 2788 | U    |
| 62  | A5    | 2789 | U    |
| 62  | A5    | 2790 | G    |
| 62  | A5    | 2797 | A    |
| 62  | A5    | 2799 | U    |
| 62  | A5    | 2806 | U    |
| 62  | A5    | 2813 | G    |
| 62  | A5    | 2816 | A    |
| 62  | A5    | 2821 | A    |
| 62  | A5    | 2822 | C    |
| 62  | A5    | 2825 | A    |
| 62  | A5    | 2828 | A    |
| 62  | A5    | 2831 | U    |
| 62  | A5    | 2832 | G    |
| 62  | A5    | 2833 | U    |
| 62  | A5    | 2834 | A    |
| 62  | A5    | 2836 | A    |
| 62  | A5    | 2837 | A    |
| 62  | A5    | 2838 | U    |
| 62  | A5    | 2839 | A    |
| 62  | A5    | 2840 | A    |
| 62  | A5    | 2842 | U    |
| 62  | A5    | 2843 | G    |
| 62  | A5    | 2847 | G    |
| 62  | A5    | 2869 | U    |
| 62  | A5    | 2870 | C    |
| 62  | A5    | 2876 | U    |
| 62  | A5    | 2877 | G    |
| 62  | A5    | 2880 | A    |
| 62  | A5    | 2881 | U    |
| 62  | A5    | 2888 | A    |
| 62  | A5    | 2891 | C    |
| 62  | A5    | 2898 | U    |
| 62  | A5    | 2899 | U    |
| 62  | A5    | 2900 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 62  | A5    | 2901 | C    |
| 62  | A5    | 2905 | A    |
| 62  | A5    | 2908 | U    |
| 62  | A5    | 2909 | A    |
| 62  | A5    | 2911 | U    |
| 62  | A5    | 2913 | G    |
| 62  | A5    | 2915 | U    |
| 62  | A5    | 2916 | U    |
| 62  | A5    | 2917 | A    |
| 62  | A5    | 2918 | A    |
| 62  | A5    | 2919 | A    |
| 62  | A5    | 2920 | U    |
| 62  | A5    | 2925 | C    |
| 62  | A5    | 2927 | U    |
| 62  | A5    | 2989 | G    |
| 62  | A5    | 2991 | A    |
| 62  | A5    | 2994 | C    |
| 62  | A5    | 2995 | U    |
| 62  | A5    | 2996 | U    |
| 62  | A5    | 2997 | C    |
| 62  | A5    | 2998 | U    |
| 62  | A5    | 2999 | U    |
| 62  | A5    | 3000 | G    |
| 62  | A5    | 3001 | A    |
| 62  | A5    | 3003 | C    |
| 62  | A5    | 3004 | A    |
| 62  | A5    | 3005 | A    |
| 62  | A5    | 3011 | C    |
| 62  | A5    | 3013 | C    |
| 62  | A5    | 3103 | U    |
| 62  | A5    | 3106 | G    |
| 62  | A5    | 3112 | A    |
| 62  | A5    | 3115 | C    |
| 62  | A5    | 3116 | A    |
| 62  | A5    | 3117 | A    |
| 62  | A5    | 3118 | U    |
| 62  | A5    | 3121 | A    |
| 62  | A5    | 3124 | G    |
| 62  | A5    | 3125 | A    |
| 62  | A5    | 3131 | C    |
| 62  | A5    | 3132 | C    |
| 62  | A5    | 3134 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 62  | A5    | 3136 | U    |
| 62  | A5    | 3138 | G    |
| 62  | A5    | 3139 | G    |
| 62  | A5    | 3143 | U    |
| 62  | A5    | 3146 | G    |
| 62  | A5    | 3149 | U    |
| 62  | A5    | 3150 | G    |
| 62  | A5    | 3151 | G    |
| 62  | A5    | 3153 | G    |
| 62  | A5    | 3155 | G    |
| 62  | A5    | 3157 | U    |
| 62  | A5    | 3158 | A    |
| 62  | A5    | 3159 | C    |
| 62  | A5    | 3160 | A    |
| 62  | A5    | 3165 | U    |
| 62  | A5    | 3167 | A    |
| 62  | A5    | 3168 | A    |
| 62  | A5    | 3170 | U    |
| 62  | A5    | 3174 | A    |
| 62  | A5    | 3180 | G    |
| 62  | A5    | 3183 | G    |
| 62  | A5    | 3184 | U    |
| 62  | A5    | 3188 | A    |
| 62  | A5    | 3189 | A    |
| 62  | A5    | 3193 | C    |
| 62  | A5    | 3195 | G    |
| 62  | A5    | 3198 | C    |
| 62  | A5    | 3200 | G    |
| 62  | A5    | 3203 | C    |
| 62  | A5    | 3204 | G    |
| 62  | A5    | 3206 | A    |
| 62  | A5    | 3208 | A    |
| 62  | A5    | 3209 | G    |
| 62  | A5    | 3210 | A    |
| 62  | A5    | 3211 | A    |
| 62  | A5    | 3212 | A    |
| 62  | A5    | 3214 | C    |
| 62  | A5    | 3217 | A    |
| 62  | A5    | 3220 | U    |
| 62  | A5    | 3221 | A    |
| 62  | A5    | 3223 | A    |
| 62  | A5    | 3226 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 62  | A5    | 3228 | A    |
| 62  | A5    | 3234 | A    |
| 62  | A5    | 3235 | A    |
| 62  | A5    | 3236 | A    |
| 62  | A5    | 3237 | U    |
| 62  | A5    | 3245 | U    |
| 62  | A5    | 3246 | G    |
| 62  | A5    | 3247 | A    |
| 62  | A5    | 3252 | G    |
| 62  | A5    | 3258 | C    |
| 62  | A5    | 3260 | G    |
| 62  | A5    | 3261 | U    |
| 62  | A5    | 3264 | A    |
| 62  | A5    | 3269 | G    |
| 62  | A5    | 3274 | A    |
| 62  | A5    | 3279 | A    |
| 62  | A5    | 3285 | G    |
| 62  | A5    | 3286 | G    |
| 62  | A5    | 3288 | C    |
| 62  | A5    | 3291 | U    |
| 62  | A5    | 3292 | C    |
| 62  | A5    | 3293 | G    |
| 62  | A5    | 3294 | A    |
| 62  | A5    | 3295 | U    |
| 62  | A5    | 3297 | C    |
| 62  | A5    | 3300 | U    |
| 62  | A5    | 3302 | G    |
| 62  | A5    | 3304 | U    |
| 62  | A5    | 3305 | U    |
| 62  | A5    | 3306 | U    |
| 62  | A5    | 3309 | A    |
| 62  | A5    | 3312 | G    |
| 62  | A5    | 3313 | U    |
| 62  | A5    | 3315 | U    |
| 62  | A5    | 3317 | U    |
| 62  | A5    | 3319 | A    |
| 62  | A5    | 3320 | C    |
| 62  | A5    | 3323 | G    |
| 62  | A5    | 3326 | G    |
| 62  | A5    | 3327 | U    |
| 62  | A5    | 3328 | G    |
| 62  | A5    | 3329 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 62  | A5    | 3331 | A    |
| 62  | A5    | 3332 | G    |
| 62  | A5    | 3333 | A    |
| 62  | A5    | 3334 | A    |
| 62  | A5    | 3336 | A    |
| 62  | A5    | 3339 | U    |
| 62  | A5    | 3340 | A    |
| 62  | A5    | 3342 | C    |
| 62  | A5    | 3343 | A    |
| 62  | A5    | 3344 | U    |
| 62  | A5    | 3345 | A    |
| 62  | A5    | 3346 | G    |
| 62  | A5    | 3348 | G    |
| 62  | A5    | 3349 | A    |
| 62  | A5    | 3350 | U    |
| 62  | A5    | 3351 | A    |
| 62  | A5    | 3355 | G    |
| 62  | A5    | 3356 | G    |
| 62  | A5    | 3359 | U    |
| 62  | A5    | 3360 | G    |
| 62  | A5    | 3362 | G    |
| 62  | A5    | 3363 | G    |
| 62  | A5    | 3368 | C    |
| 62  | A5    | 3374 | U    |
| 62  | A5    | 3377 | A    |
| 62  | A5    | 3379 | A    |
| 62  | A5    | 3381 | C    |
| 62  | A5    | 3382 | G    |
| 62  | A5    | 3389 | C    |
| 62  | A5    | 3394 | U    |
| 62  | A5    | 3395 | G    |
| 62  | A5    | 3396 | A    |
| 62  | A5    | 3397 | U    |
| 62  | A5    | 3399 | C    |
| 62  | A5    | 3403 | G    |
| 62  | A5    | 3404 | A    |
| 62  | A5    | 3410 | G    |
| 62  | A5    | 3411 | C    |
| 62  | A5    | 3414 | U    |
| 62  | A5    | 3415 | U    |
| 62  | A5    | 3418 | U    |
| 62  | A5    | 3423 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 62  | A5    | 3431 | C    |
| 62  | A5    | 3441 | C    |
| 62  | A5    | 3443 | A    |
| 62  | A5    | 3444 | G    |
| 62  | A5    | 3445 | C    |
| 62  | A5    | 3447 | U    |
| 62  | A5    | 3448 | U    |
| 62  | A5    | 3453 | U    |
| 62  | A5    | 3454 | G    |
| 62  | A5    | 3456 | U    |
| 62  | A5    | 3460 | C    |
| 62  | A5    | 3461 | C    |
| 62  | A5    | 3465 | C    |
| 62  | A5    | 3466 | A    |
| 62  | A5    | 3468 | G    |
| 62  | A5    | 3471 | A    |
| 62  | A5    | 3472 | A    |
| 62  | A5    | 3473 | C    |
| 62  | A5    | 3474 | G    |
| 62  | A5    | 3475 | U    |
| 62  | A5    | 3477 | A    |
| 62  | A5    | 3481 | G    |
| 62  | A5    | 3482 | G    |
| 62  | A5    | 3485 | U    |
| 62  | A5    | 3486 | U    |
| 62  | A5    | 3488 | G    |
| 62  | A5    | 3492 | G    |
| 62  | A5    | 3497 | G    |
| 62  | A5    | 3498 | A    |
| 62  | A5    | 3499 | G    |
| 62  | A5    | 3500 | A    |
| 62  | A5    | 3501 | C    |
| 62  | A5    | 3502 | A    |
| 62  | A5    | 3505 | U    |
| 62  | A5    | 3506 | U    |
| 62  | A5    | 3508 | G    |
| 62  | A5    | 3510 | U    |
| 62  | A5    | 3511 | U    |
| 62  | A5    | 3514 | C    |
| 62  | A5    | 3515 | C    |
| 62  | A5    | 3516 | C    |
| 62  | A5    | 3517 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 62  | A5    | 3521 | A    |
| 62  | A5    | 3527 | A    |
| 62  | A5    | 3531 | C    |
| 62  | A5    | 3532 | G    |
| 62  | A5    | 3535 | G    |
| 62  | A5    | 3539 | C    |
| 62  | A5    | 3541 | A    |
| 62  | A5    | 3542 | C    |
| 62  | A5    | 3544 | G    |
| 62  | A5    | 3546 | A    |
| 62  | A5    | 3547 | U    |
| 62  | A5    | 3550 | C    |
| 62  | A5    | 3554 | G    |
| 62  | A5    | 3556 | A    |
| 62  | A5    | 3557 | G    |
| 62  | A5    | 3558 | U    |
| 62  | A5    | 3568 | A    |
| 62  | A5    | 3569 | C    |
| 62  | A5    | 3575 | G    |
| 62  | A5    | 3579 | C    |
| 62  | A5    | 3581 | G    |
| 62  | A5    | 3582 | A    |
| 62  | A5    | 3583 | C    |
| 62  | A5    | 3585 | A    |
| 62  | A5    | 3589 | G    |
| 62  | A5    | 3590 | C    |
| 62  | A5    | 3591 | A    |
| 62  | A5    | 3592 | C    |
| 62  | A5    | 3593 | A    |
| 62  | A5    | 3594 | A    |
| 62  | A5    | 3595 | U    |
| 62  | A5    | 3596 | A    |
| 62  | A5    | 3602 | U    |
| 62  | A5    | 3604 | G    |
| 62  | A5    | 3606 | G    |
| 62  | A5    | 3608 | G    |
| 62  | A5    | 3609 | A    |
| 62  | A5    | 3610 | A    |
| 62  | A5    | 3611 | C    |
| 62  | A5    | 3613 | G    |
| 62  | A5    | 3614 | U    |
| 62  | A5    | 3615 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 62  | A5    | 3616 | G    |
| 62  | A5    | 3621 | A    |
| 62  | A5    | 3623 | G    |
| 62  | A5    | 3627 | C    |
| 62  | A5    | 3628 | G    |
| 62  | A5    | 3637 | A    |
| 62  | A5    | 3638 | U    |
| 62  | A5    | 3639 | U    |
| 62  | A5    | 3640 | A    |
| 62  | A5    | 3641 | U    |
| 62  | A5    | 3642 | G    |
| 62  | A5    | 3643 | C    |
| 62  | A5    | 3649 | C    |
| 62  | A5    | 3650 | G    |
| 62  | A5    | 3652 | C    |
| 62  | A5    | 3655 | U    |
| 62  | A5    | 3656 | A    |
| 62  | A5    | 3657 | A    |
| 62  | A5    | 3659 | G    |
| 62  | A5    | 3664 | A    |
| 62  | A5    | 3665 | U    |
| 62  | A5    | 3666 | C    |
| 62  | A5    | 3667 | C    |
| 62  | A5    | 3670 | G    |
| 62  | A5    | 3672 | U    |
| 62  | A5    | 3673 | G    |
| 62  | A5    | 3675 | A    |
| 62  | A5    | 3676 | C    |
| 62  | A5    | 3677 | U    |
| 62  | A5    | 3678 | G    |
| 62  | A5    | 3679 | C    |
| 62  | A5    | 3681 | A    |
| 62  | A5    | 3684 | A    |
| 62  | A5    | 3685 | U    |
| 62  | A5    | 3686 | A    |
| 62  | A5    | 3688 | A    |
| 62  | A5    | 3689 | U    |
| 62  | A5    | 3690 | A    |
| 62  | A5    | 3696 | C    |
| 62  | A5    | 3697 | A    |
| 62  | A5    | 3698 | A    |
| 62  | A5    | 3699 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 62  | A5    | 3701 | U    |
| 62  | A5    | 3702 | G    |
| 62  | A5    | 3709 | A    |
| 62  | A5    | 3710 | U    |
| 62  | A5    | 3711 | G    |
| 62  | A5    | 3712 | G    |
| 62  | A5    | 3713 | C    |
| 62  | A5    | 3715 | U    |
| 62  | A5    | 3716 | C    |
| 62  | A5    | 3717 | U    |
| 62  | A5    | 3718 | A    |
| 62  | A5    | 3719 | A    |
| 62  | A5    | 3720 | A    |
| 62  | A5    | 3722 | C    |
| 62  | A5    | 3723 | A    |
| 62  | A5    | 3724 | U    |
| 62  | A5    | 3725 | U    |
| 62  | A5    | 3726 | U    |
| 62  | A5    | 3728 | A    |
| 62  | A5    | 3729 | A    |
| 62  | A5    | 3730 | G    |
| 62  | A5    | 3735 | U    |
| 62  | A5    | 3742 | C    |
| 62  | A5    | 3743 | U    |
| 62  | A5    | 3749 | A    |
| 62  | A5    | 3752 | G    |
| 62  | A5    | 3753 | A    |
| 62  | A5    | 3754 | C    |
| 62  | A5    | 3755 | A    |
| 62  | A5    | 3756 | A    |
| 62  | A5    | 3757 | U    |
| 62  | A5    | 3758 | G    |
| 62  | A5    | 3759 | G    |
| 62  | A5    | 3760 | A    |
| 62  | A5    | 3761 | U    |
| 62  | A5    | 3762 | G    |
| 62  | A5    | 3763 | U    |
| 62  | A5    | 3764 | G    |
| 62  | A5    | 3765 | A    |
| 62  | A5    | 3766 | U    |
| 62  | A5    | 3767 | G    |
| 62  | A5    | 3768 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 62  | A5    | 3770 | A    |
| 62  | A5    | 3771 | A    |
| 62  | A5    | 3772 | U    |
| 62  | A5    | 3773 | G    |
| 62  | A5    | 3774 | U    |
| 62  | A5    | 3775 | A    |
| 62  | A5    | 3776 | A    |
| 62  | A5    | 3779 | U    |
| 62  | A5    | 3780 | G    |
| 62  | A5    | 3785 | A    |
| 62  | A5    | 3789 | U    |
| 62  | A5    | 3791 | A    |
| 62  | A5    | 3794 | U    |
| 62  | A5    | 3795 | G    |
| 62  | A5    | 3798 | A    |
| 62  | A5    | 3801 | A    |
| 62  | A5    | 3802 | U    |
| 62  | A5    | 3803 | C    |
| 62  | A5    | 3805 | U    |
| 62  | A5    | 3806 | C    |
| 62  | A5    | 3808 | A    |
| 62  | A5    | 3809 | U    |
| 62  | A5    | 3811 | A    |
| 62  | A5    | 3818 | G    |
| 62  | A5    | 3819 | C    |
| 62  | A5    | 3820 | C    |
| 62  | A5    | 3821 | G    |
| 62  | A5    | 3822 | C    |
| 62  | A5    | 3823 | G    |
| 62  | A5    | 3824 | C    |
| 62  | A5    | 3833 | U    |
| 62  | A5    | 3839 | A    |
| 62  | A5    | 3840 | G    |
| 62  | A5    | 3841 | C    |
| 62  | A5    | 3844 | U    |
| 62  | A5    | 3845 | A    |
| 62  | A5    | 3846 | U    |
| 62  | A5    | 3847 | U    |
| 62  | A5    | 3849 | A    |
| 62  | A5    | 3850 | A    |
| 62  | A5    | 3852 | A    |
| 62  | A5    | 3856 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 62  | A5    | 3860 | A    |
| 62  | A5    | 3861 | A    |
| 62  | A5    | 3862 | A    |
| 62  | A5    | 3867 | A    |
| 62  | A5    | 3868 | G    |
| 62  | A5    | 3869 | A    |
| 62  | A5    | 3872 | C    |
| 62  | A5    | 3875 | U    |
| 62  | A5    | 3876 | U    |
| 62  | A5    | 3878 | U    |
| 62  | A5    | 3879 | A    |
| 62  | A5    | 3882 | C    |
| 62  | A5    | 3883 | G    |
| 62  | A5    | 3884 | A    |
| 62  | A5    | 3887 | U    |
| 62  | A5    | 3889 | U    |
| 62  | A5    | 3890 | G    |
| 62  | A5    | 3891 | U    |
| 62  | A5    | 3892 | A    |
| 62  | A5    | 3893 | A    |
| 62  | A5    | 3894 | C    |
| 62  | A5    | 3898 | C    |
| 62  | A5    | 3899 | A    |
| 62  | A5    | 3901 | G    |
| 62  | A5    | 3904 | G    |
| 62  | A5    | 3906 | U    |
| 62  | A5    | 3907 | G    |
| 62  | A5    | 3908 | U    |
| 62  | A5    | 3910 | A    |
| 62  | A5    | 3912 | U    |
| 62  | A5    | 3916 | U    |
| 62  | A5    | 3917 | G    |
| 62  | A5    | 3918 | A    |
| 62  | A5    | 3919 | G    |
| 62  | A5    | 3921 | A    |
| 62  | A5    | 3923 | C    |
| 62  | A5    | 3924 | U    |
| 62  | A5    | 3925 | G    |
| 62  | A5    | 3926 | C    |
| 62  | A5    | 3928 | A    |
| 62  | A5    | 3929 | U    |
| 62  | A5    | 3932 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 62  | A5    | 3933 | G    |
| 62  | A5    | 3935 | G    |
| 62  | A5    | 3936 | A    |
| 62  | A5    | 3937 | U    |
| 62  | A5    | 3943 | G    |
| 62  | A5    | 3949 | U    |
| 62  | A5    | 3950 | A    |
| 62  | A5    | 3952 | C    |
| 62  | A5    | 3955 | U    |
| 62  | A5    | 3956 | U    |
| 62  | A5    | 3958 | C    |
| 62  | A5    | 3959 | U    |
| 62  | A5    | 3960 | U    |
| 62  | A5    | 3961 | G    |
| 62  | A5    | 3962 | A    |
| 62  | A5    | 3963 | U    |
| 62  | A5    | 3964 | G    |
| 62  | A5    | 3965 | A    |
| 62  | A5    | 3969 | G    |
| 81  | B     | 3    | C    |
| 81  | B     | 5    | G    |
| 81  | B     | 8    | U    |
| 81  | B     | 9    | G    |
| 81  | B     | 10   | G    |
| 81  | B     | 13   | C    |
| 81  | B     | 16   | U    |
| 81  | B     | 17   | G    |
| 81  | B     | 18   | G    |
| 81  | B     | 19   | A    |
| 81  | B     | 20   | A    |
| 81  | B     | 21   | G    |
| 81  | B     | 25   | G    |
| 81  | B     | 33   | C    |
| 81  | B     | 34   | A    |
| 81  | B     | 45   | G    |
| 81  | B     | 46   | U    |
| 81  | B     | 47   | C    |
| 81  | B     | 48   | C    |
| 81  | B     | 51   | G    |
| 81  | B     | 58   | A    |
| 81  | B     | 60   | C    |
| 81  | B     | 71   | U    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 81  | B     | 72  | A    |
| 81  | B     | 73  | C    |
| 81  | B     | 74  | C    |
| 81  | B     | 75  | A    |
| 82  | v     | 26  | G    |
| 82  | v     | 29  | G    |
| 82  | v     | 32  | G    |
| 82  | v     | 34  | C    |
| 82  | v     | 35  | C    |
| 82  | v     | 36  | U    |

All (117) RNA pucker outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 57  | A9    | 21   | G    |
| 58  | A7    | 119  | C    |
| 59  | A8    | 101  | A    |
| 59  | A8    | 109  | U    |
| 61  | B2    | 172  | G    |
| 61  | B2    | 248  | G    |
| 61  | B2    | 250  | U    |
| 61  | B2    | 251  | G    |
| 61  | B2    | 256  | C    |
| 61  | B2    | 278  | G    |
| 61  | B2    | 378  | G    |
| 61  | B2    | 381  | C    |
| 61  | B2    | 422  | A    |
| 61  | B2    | 488  | A    |
| 61  | B2    | 511  | G    |
| 61  | B2    | 563  | A    |
| 61  | B2    | 878  | C    |
| 61  | B2    | 1138 | U    |
| 61  | B2    | 1186 | U    |
| 61  | B2    | 1250 | C    |
| 61  | B2    | 1310 | A    |
| 61  | B2    | 1448 | A    |
| 61  | B2    | 1547 | U    |
| 61  | B2    | 1594 | A    |
| 61  | B2    | 1673 | U    |
| 61  | B2    | 1765 | U    |
| 61  | B2    | 1849 | U    |
| 61  | B2    | 1881 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 61  | B2    | 1949 | A    |
| 61  | B2    | 1956 | U    |
| 62  | A5    | 17   | C    |
| 62  | A5    | 99   | A    |
| 62  | A5    | 175  | U    |
| 62  | A5    | 186  | G    |
| 62  | A5    | 197  | G    |
| 62  | A5    | 225  | U    |
| 62  | A5    | 272  | U    |
| 62  | A5    | 356  | A    |
| 62  | A5    | 463  | C    |
| 62  | A5    | 552  | U    |
| 62  | A5    | 580  | A    |
| 62  | A5    | 615  | C    |
| 62  | A5    | 620  | U    |
| 62  | A5    | 640  | U    |
| 62  | A5    | 641  | A    |
| 62  | A5    | 670  | G    |
| 62  | A5    | 748  | A    |
| 62  | A5    | 797  | A    |
| 62  | A5    | 872  | A    |
| 62  | A5    | 874  | G    |
| 62  | A5    | 999  | U    |
| 62  | A5    | 1070 | G    |
| 62  | A5    | 1080 | G    |
| 62  | A5    | 1094 | A    |
| 62  | A5    | 1095 | G    |
| 62  | A5    | 1096 | A    |
| 62  | A5    | 1143 | U    |
| 62  | A5    | 1161 | C    |
| 62  | A5    | 1231 | A    |
| 62  | A5    | 1277 | A    |
| 62  | A5    | 1306 | G    |
| 62  | A5    | 1310 | A    |
| 62  | A5    | 1330 | G    |
| 62  | A5    | 1357 | C    |
| 62  | A5    | 1368 | A    |
| 62  | A5    | 1374 | C    |
| 62  | A5    | 1382 | U    |
| 62  | A5    | 1394 | U    |
| 62  | A5    | 1395 | U    |
| 62  | A5    | 1516 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 62  | A5    | 1523 | A    |
| 62  | A5    | 1594 | U    |
| 62  | A5    | 1688 | A    |
| 62  | A5    | 1784 | A    |
| 62  | A5    | 1801 | U    |
| 62  | A5    | 1873 | A    |
| 62  | A5    | 1960 | C    |
| 62  | A5    | 2002 | C    |
| 62  | A5    | 2028 | A    |
| 62  | A5    | 2126 | A    |
| 62  | A5    | 2129 | C    |
| 62  | A5    | 2158 | U    |
| 62  | A5    | 2182 | G    |
| 62  | A5    | 2201 | U    |
| 62  | A5    | 2222 | G    |
| 62  | A5    | 2702 | A    |
| 62  | A5    | 2782 | A    |
| 62  | A5    | 2868 | A    |
| 62  | A5    | 2904 | U    |
| 62  | A5    | 2919 | A    |
| 62  | A5    | 2990 | C    |
| 62  | A5    | 2993 | G    |
| 62  | A5    | 3017 | U    |
| 62  | A5    | 3260 | G    |
| 62  | A5    | 3393 | U    |
| 62  | A5    | 3396 | A    |
| 62  | A5    | 3473 | C    |
| 62  | A5    | 3481 | G    |
| 62  | A5    | 3485 | U    |
| 62  | A5    | 3516 | C    |
| 62  | A5    | 3567 | A    |
| 62  | A5    | 3591 | A    |
| 62  | A5    | 3627 | C    |
| 62  | A5    | 3676 | C    |
| 62  | A5    | 3678 | G    |
| 62  | A5    | 3697 | A    |
| 62  | A5    | 3708 | U    |
| 62  | A5    | 3714 | U    |
| 62  | A5    | 3762 | G    |
| 62  | A5    | 3765 | A    |
| 62  | A5    | 3808 | A    |
| 62  | A5    | 3844 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 62  | A5    | 3890 | G    |
| 62  | A5    | 3891 | U    |
| 62  | A5    | 3949 | U    |
| 62  | A5    | 3961 | G    |
| 81  | B     | 18   | G    |

## 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](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 61  | B2    | 2                |
| 62  | A5    | 2                |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | B2    | 1236:C    | O3'    | 1237:G    | P      | 6.91         |
| 1     | A5    | 2896:U    | O3'    | 2897:G    | P      | 5.92         |
| 1     | B2    | 1817:C    | O3'    | 1818:U    | P      | 4.83         |
| 1     | A5    | 2819:A    | O3'    | 2820:G    | P      | 3.80         |

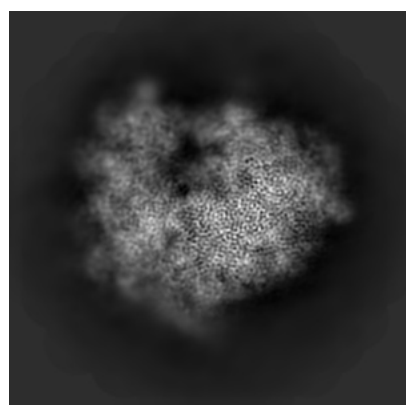
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10623. These allow visual inspection of the internal detail of the map and identification of artifacts.

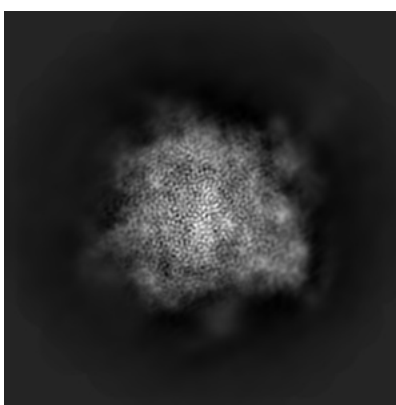
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

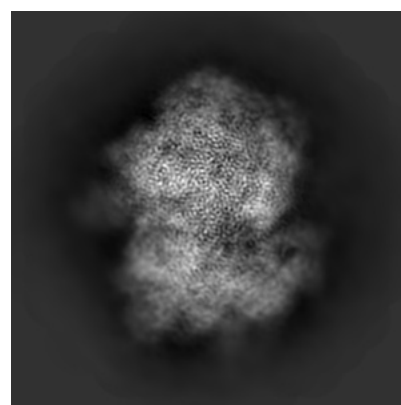
#### 6.1.1 Primary map



X



Y

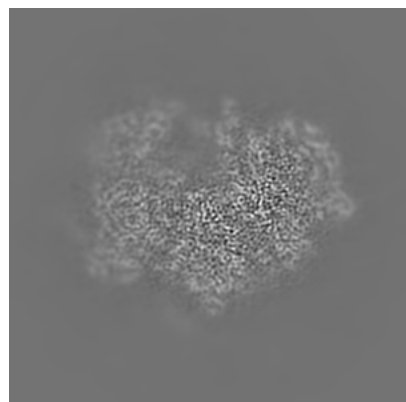


Z

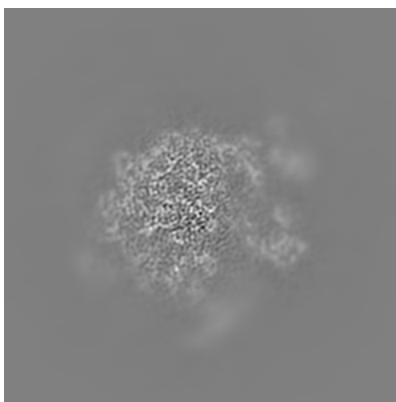
The images above show the map projected in three orthogonal directions.

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

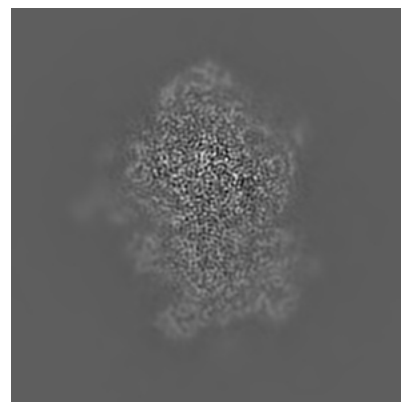
#### 6.2.1 Primary map



X Index: 200



Y Index: 200

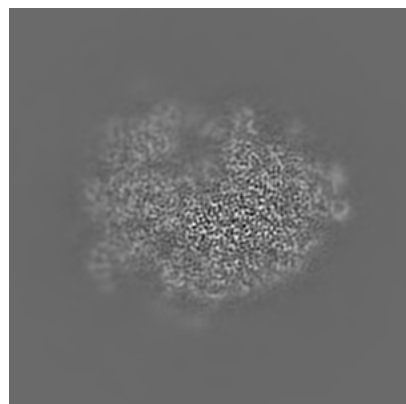


Z Index: 200

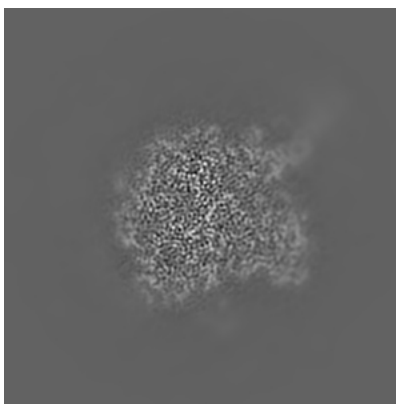
The images above show central slices of the map in three orthogonal directions.

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

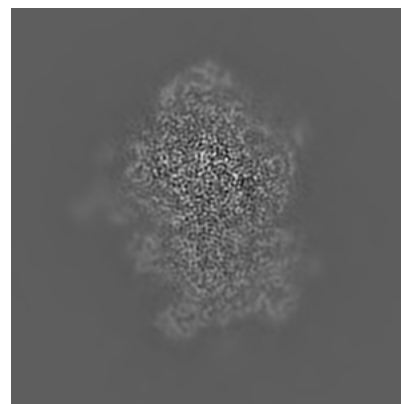
### 6.3.1 Primary map



X Index: 185



Y Index: 230

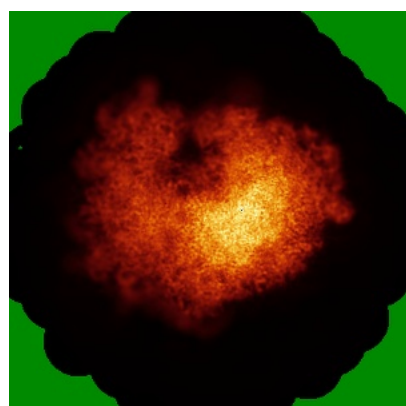


Z Index: 200

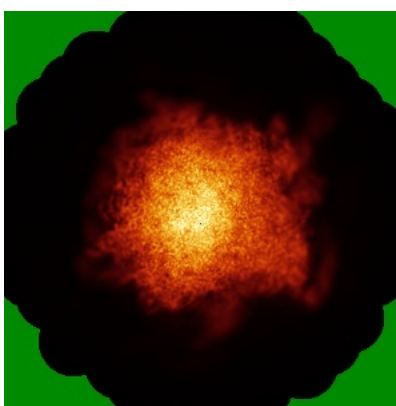
The images above show the largest variance slices of the map in three orthogonal directions.

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

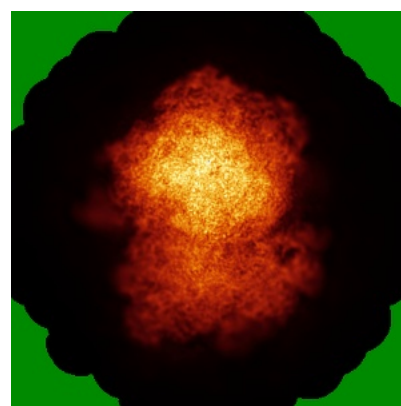
### 6.4.1 Primary map



X



Y



Z

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

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

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.035. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

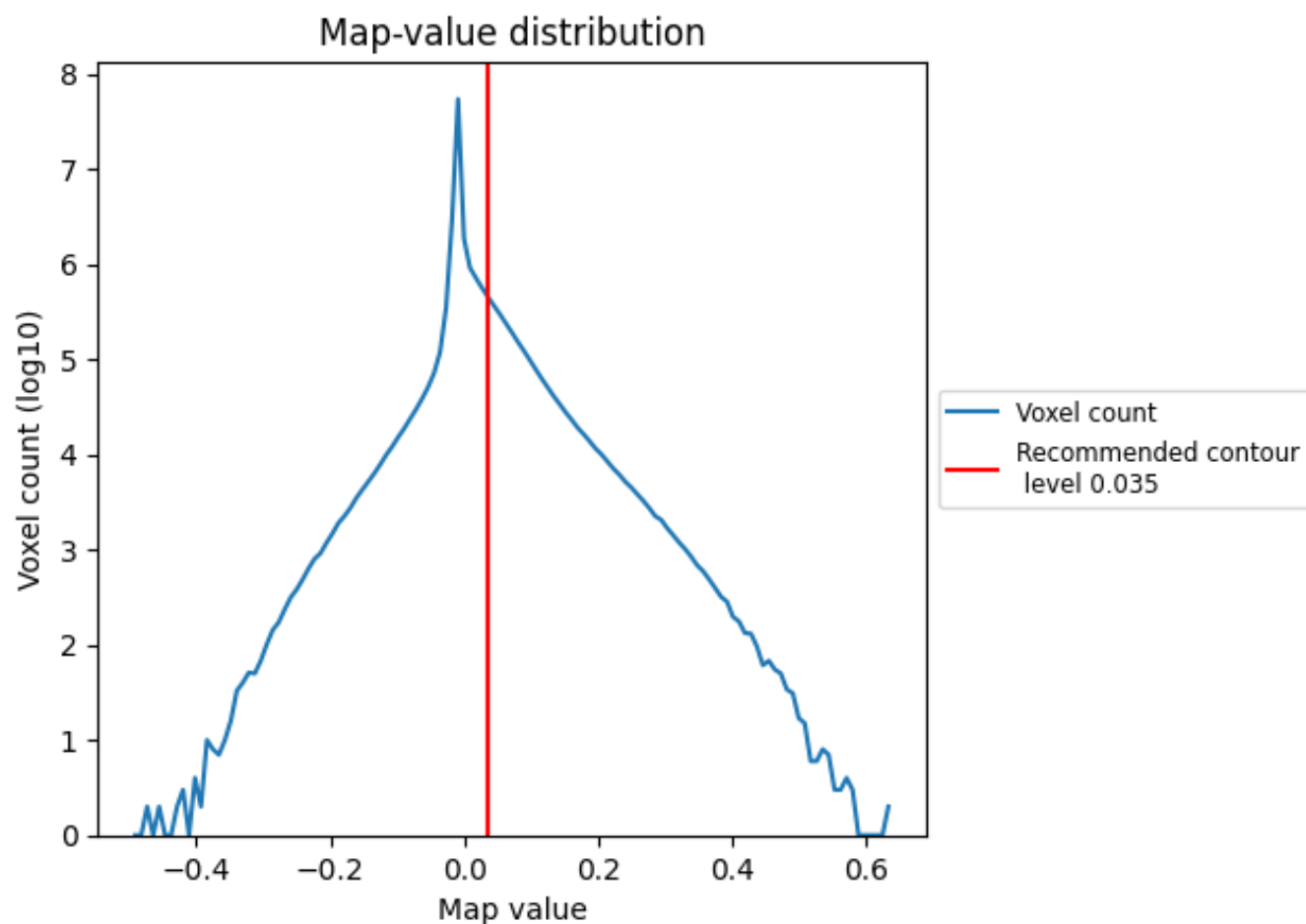
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

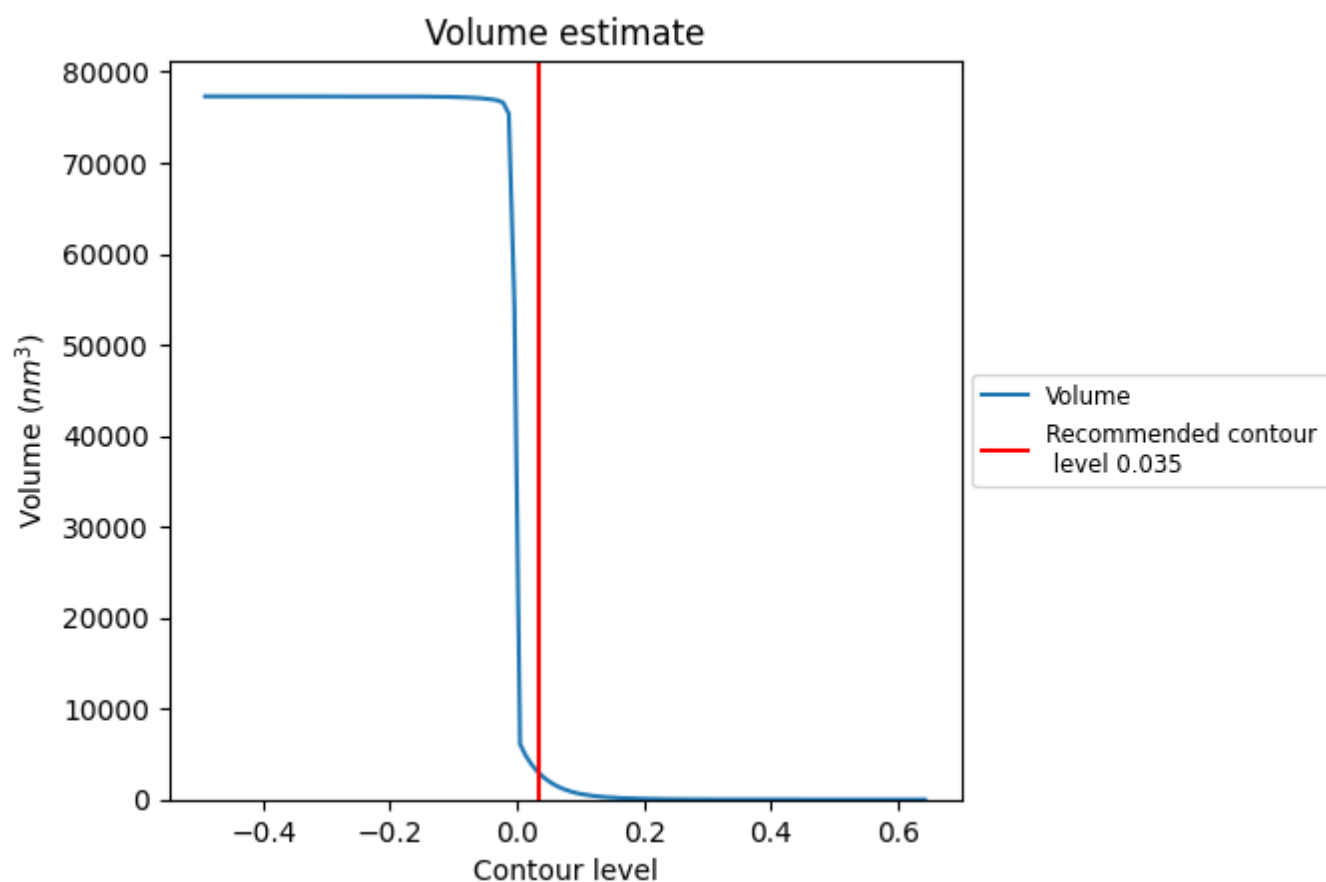
This section contains the results of statistical analysis of the map.

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



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

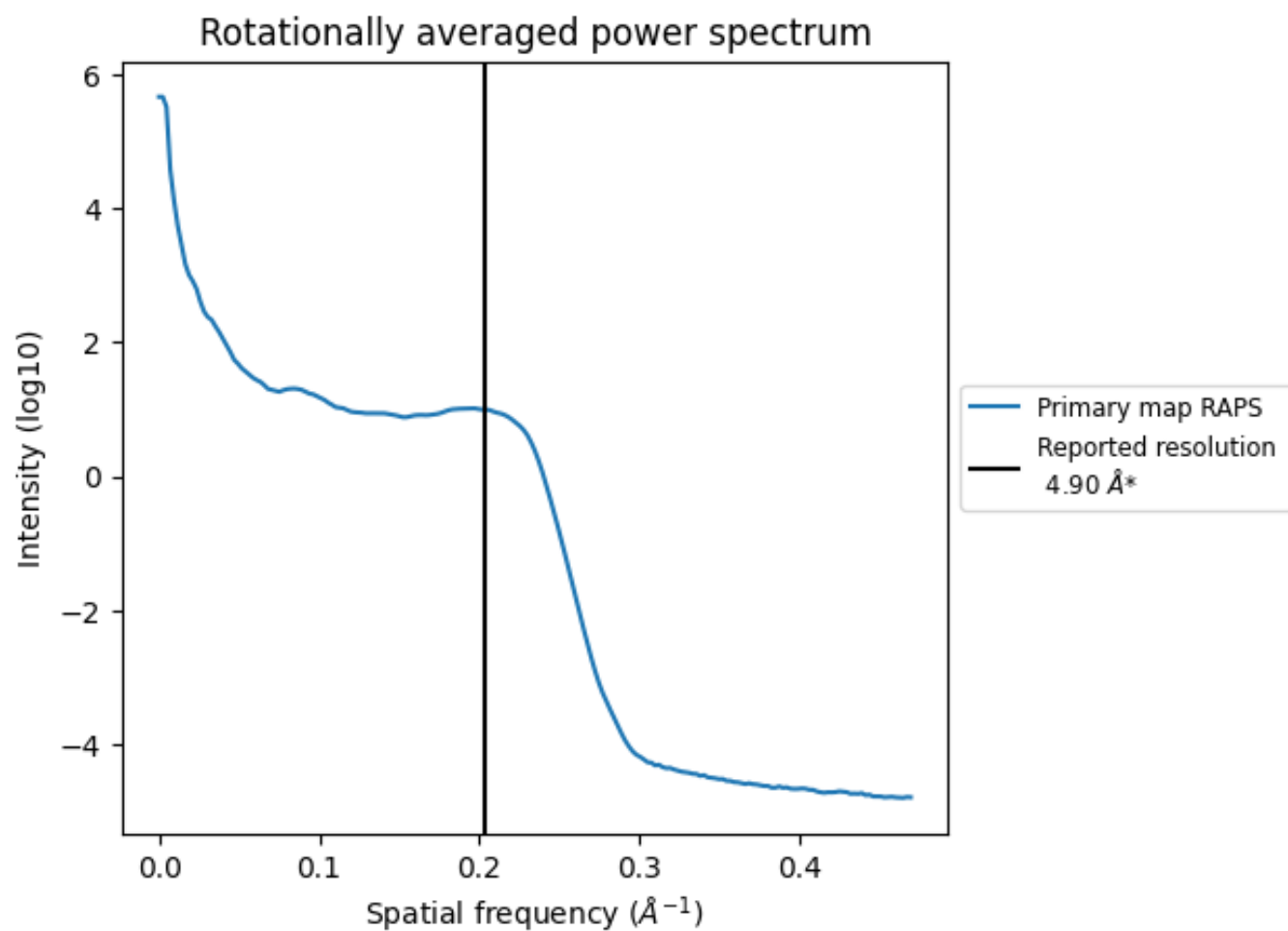
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2920 nm<sup>3</sup>; this corresponds to an approximate mass of 2638 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 ⓘ

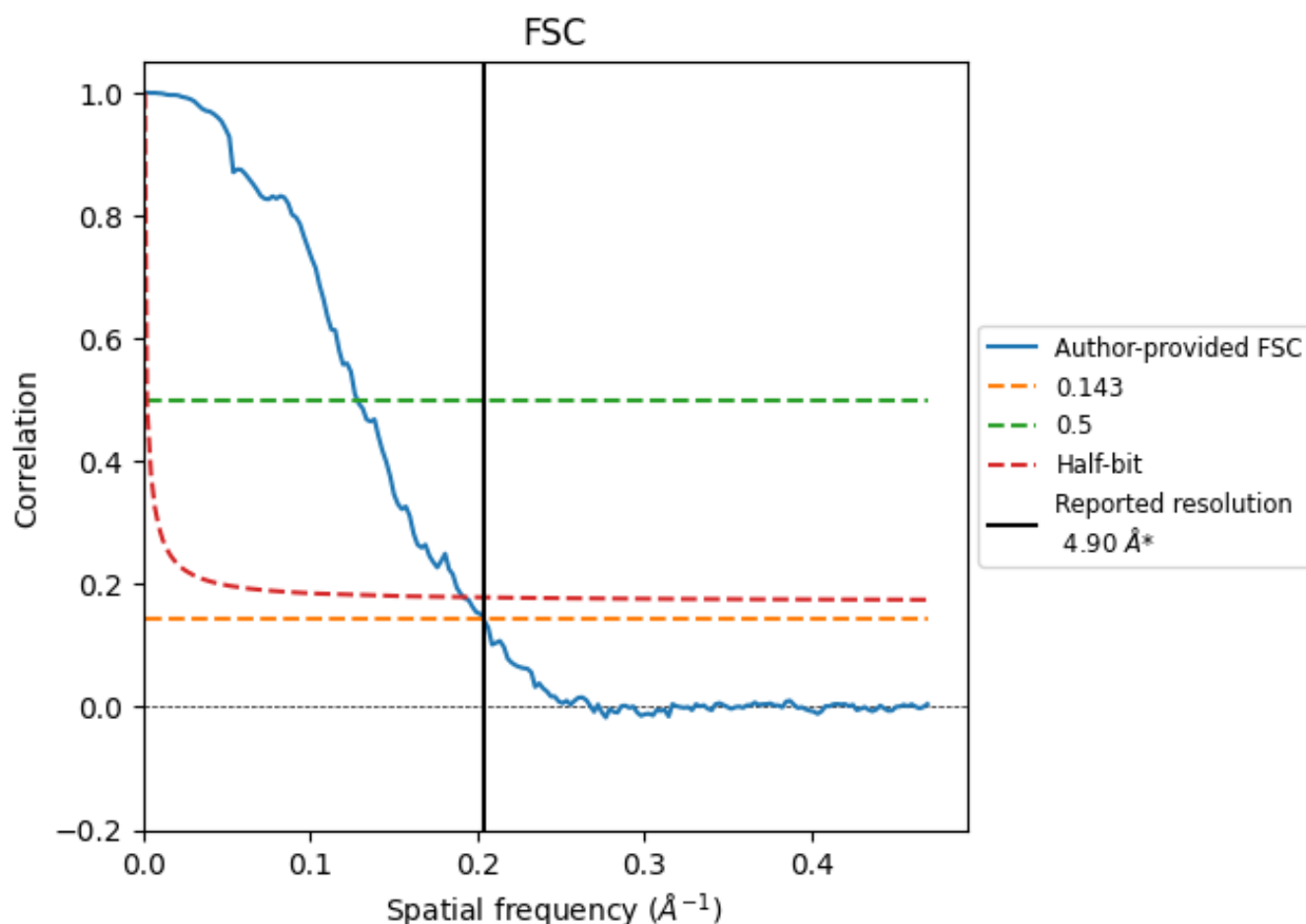


\*Reported resolution corresponds to spatial frequency of 0.204 Å<sup>-1</sup>

## 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 0.204 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

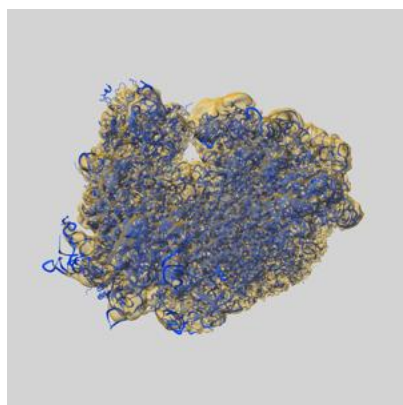
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 4.90                               | -    | -        |
| Author-provided FSC curve | 4.91                               | 7.80 | 5.21     |
| Unmasked-calculated*      | -                                  | -    | -        |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

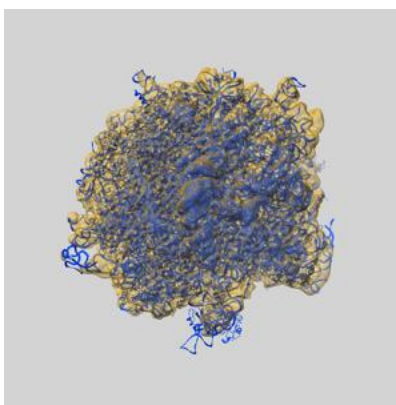
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-10623 and PDB model 6XU7. Per-residue inclusion information can be found in [section 3](#) on [page 20](#).

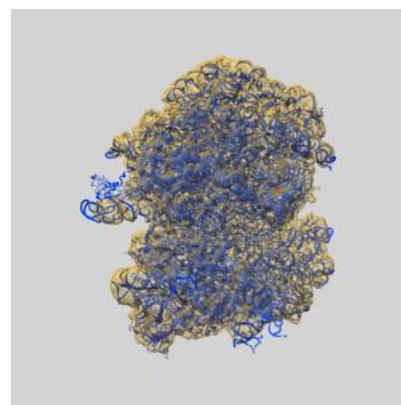
### 9.1 Map-model overlay [i](#)



X



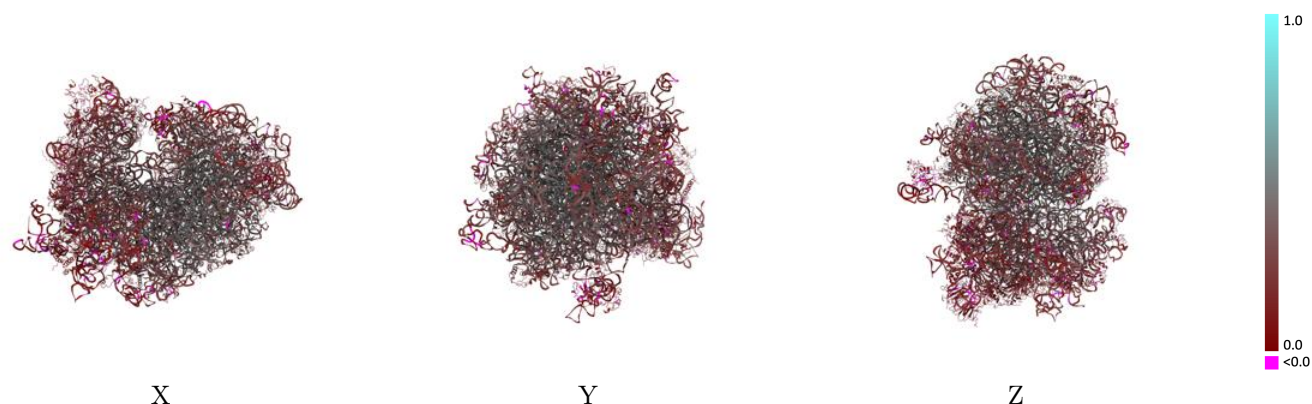
Y



Z

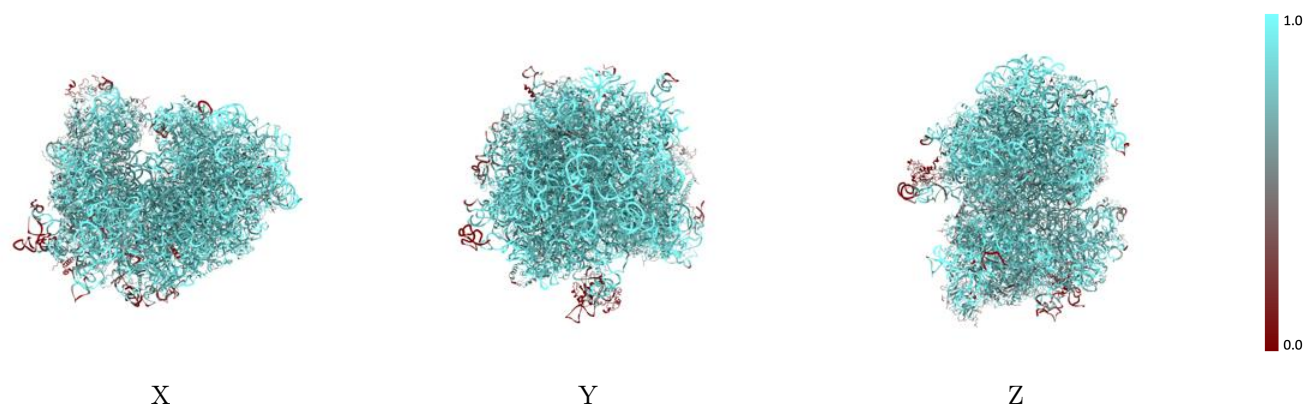
The images above show the 3D surface view of the map at the recommended contour level 0.035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



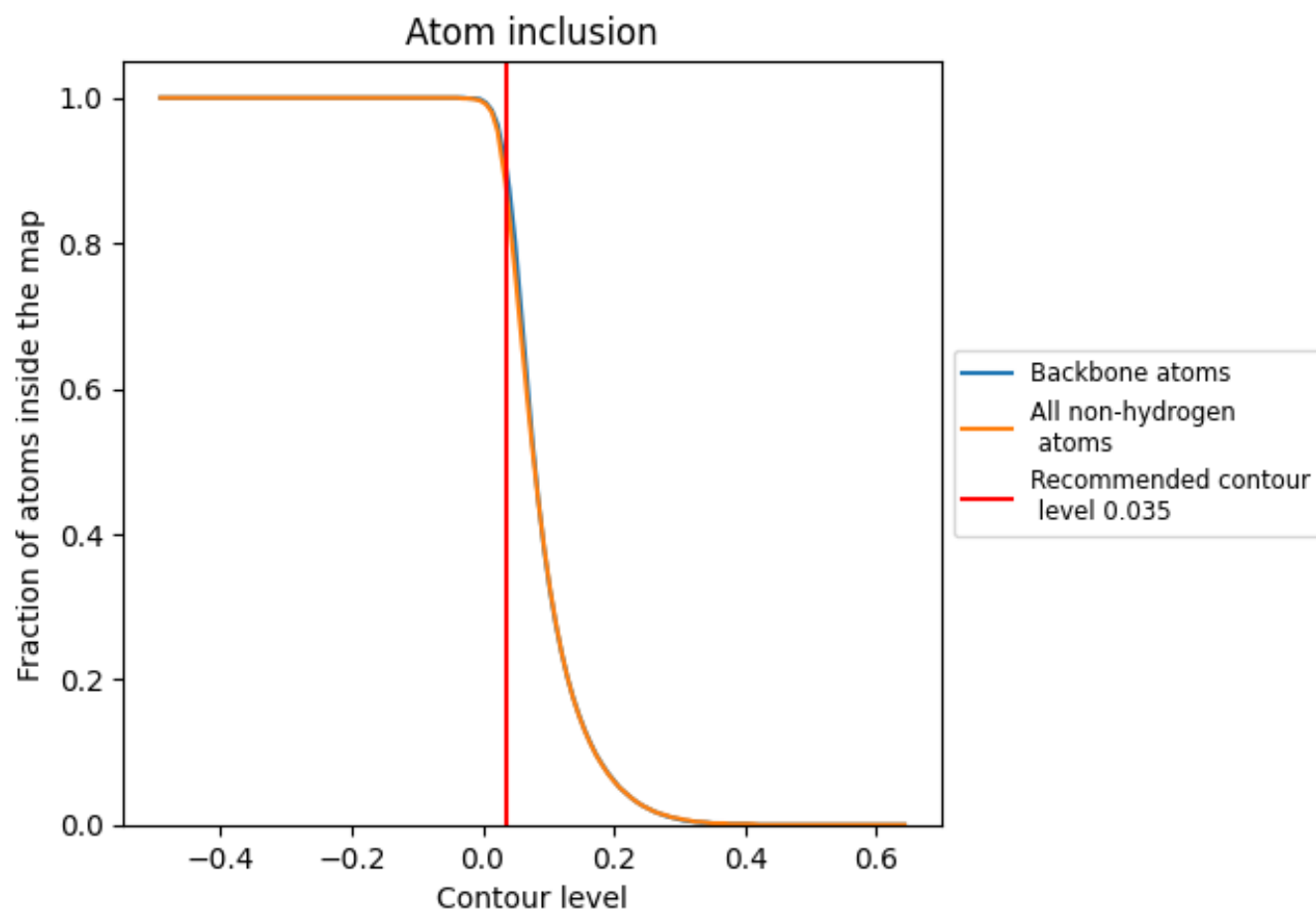
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.035).

## 9.4 Atom inclusion ⓘ



At the recommended contour level, 91% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.035) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.8820   |  0.3080   |
| A5    |  0.9390   |  0.3480   |
| A7    |  0.9890   |  0.3240   |
| A8    |  0.9720   |  0.3830   |
| A9    |  0.9940   |  0.3590   |
| AA    |  0.7250   |  0.1960   |
| AB    |  0.7430   |  0.2320   |
| AC    |  0.7880   |  0.2630   |
| AD    |  0.6780   |  0.2180   |
| AE    |  0.7870   |  0.2180   |
| AF    |  0.7630   |  0.1920   |
| AG    |  0.7640   |  0.1780   |
| AH    |  0.6970   |  0.1920   |
| AI    |  0.7830   |  0.2500   |
| AJ    |  0.8010  |  0.2180  |
| AK    |  0.7470 |  0.1760 |
| AL    |  0.7060 |  0.3020 |
| AM    |  0.3330 |  0.1230 |
| AN    |  0.8460 |  0.3200 |
| AO    |  0.7320 |  0.2370 |
| AP    |  0.6860 |  0.1630 |
| AQ    |  0.7640 |  0.1890 |
| AR    |  0.7050 |  0.2090 |
| AS    |  0.7850 |  0.1830 |
| AT    |  0.8010 |  0.1720 |
| AU    |  0.7190 |  0.2050 |
| AV    |  0.7740 |  0.2390 |
| AW    |  0.8310 |  0.2850 |
| AX    |  0.8320 |  0.3320 |
| AY    |  0.8000 |  0.1660 |
| AZ    |  0.7260 |  0.1800 |
| Aa    |  0.8040 |  0.3290 |
| Ab    |  0.7400 |  0.2020 |
| Ac    |  0.7140 |  0.1970 |
| Ad    |  0.8330 |  0.2120 |



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| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| Ae    |  0.7020   |  0.2000   |
| Af    |  0.5090   |  0.1050   |
| Ag    |  0.7050   |  0.1460   |
| B     |  0.8550   |  0.2680   |
| B2    |  0.9250   |  0.2690   |
| CA    |  0.8970   |  0.4180   |
| CB    |  0.8970   |  0.3910   |
| CC    |  0.9160   |  0.3880   |
| CD    |  0.8990   |  0.2520   |
| CE    |  0.8220   |  0.2310   |
| CF    |  0.9140   |  0.3860   |
| CG    |  0.7960   |  0.2770   |
| CH    |  0.8880   |  0.3040   |
| CI    |  0.8420   |  0.2940   |
| CJ    |  0.8380   |  0.2010   |
| CL    |  0.8480   |  0.3380   |
| CM    |  0.8290   |  0.2520   |
| CN    |  0.9360   |  0.4350   |
| CO    |  0.9080   |  0.3830   |
| CP    |  0.8190  |  0.3910  |
| CQ    |  0.9350 |  0.4110 |
| CR    |  0.8130 |  0.3440 |
| CS    |  0.9050 |  0.3690 |
| CT    |  0.8940 |  0.3790 |
| CU    |  0.8670 |  0.2630 |
| CV    |  0.9170 |  0.4190 |
| CW    |  0.9320 |  0.4200 |
| CX    |  0.9050 |  0.3560 |
| CY    |  0.9490 |  0.3710 |
| CZ    |  0.8870 |  0.2720 |
| Ca    |  0.9270 |  0.3950 |
| Cb    |  0.9280 |  0.3540 |
| Cc    |  0.8360 |  0.3230 |
| Cd    |  0.9240 |  0.4240 |
| Ce    |  0.9310 |  0.4550 |
| Cf    |  0.8970 |  0.3430 |
| Cg    |  0.8780 |  0.3680 |
| Ch    |  0.9160 |  0.3560 |
| Ci    |  0.8250 |  0.3000 |
| Cj    |  0.8840 |  0.4040 |
| Ck    |  0.8620 |  0.2850 |
| Cl    |  0.9300 |  0.4490 |

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| Chain | Atom inclusion                                                                           | Q-score                                                                                  |
|-------|------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------|
| Cm    |  0.8530 |  0.3090 |
| Cn    |  0.9440 |  0.4660 |
| Co    |  0.8880 |  0.3730 |
| Cp    |  0.9050 |  0.4040 |
| Cr    |  0.8510 |  0.3230 |
| Cz    |  0.0410 |  0.0690 |
| v     |  0.8750 |  0.3200 |