



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 12:57 am BST

PDB ID : 4U24  
Title : Crystal structure of the E. coli ribosome bound to dalfopristin.  
Authors : Noeske, J.; Huang, J.; Olivier, N.B.; Giacobbe, R.A.; Zambrowski, M.; Cate, J.H.D.  
Deposited on : 2014-07-16  
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

|                                |   |  |
|--------------------------------|---|--|
| MolProbity                     | : | 4.02b-467  |
| Mogul                          | : | 1.8.5 (274361), CSD as541be (2020)                                 |
| Xtriage (Phenix)               | : | 1.13   |
| EDS                            | : | 2.11   |
| buster-report                  | : | 1.1.7 (2018)   |
| Percentile statistics          | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Refmac                         | : | 5.8.0158   |
| CCP4                           | : | 7.0.044 (Gargrove)   |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)  |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)  |
| Validation Pipeline (wwPDB-VP) | : | 2.11   |

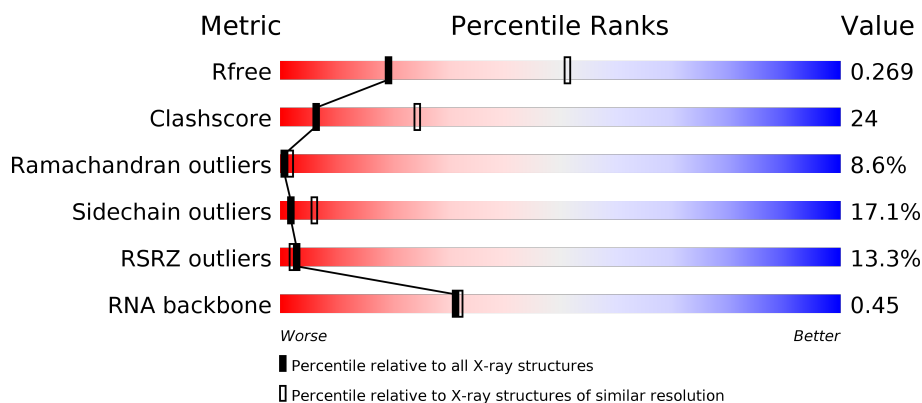
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 130704                      | 1957 (2.90-2.90)                                      |
| Clashscore            | 141614                      | 2172 (2.90-2.90)                                      |
| Ramachandran outliers | 138981                      | 2115 (2.90-2.90)                                      |
| Sidechain outliers    | 138945                      | 2117 (2.90-2.90)                                      |
| RSRZ outliers         | 127900                      | 1906 (2.90-2.90)                                      |
| RNA backbone          | 3102                        | 1007 (3.16-2.64)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower 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 electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain                                      |
|-----|-------|--------|---|
| 1   | AA    | 1539   | <div> <div>2%</div> <div>30% 54% 16%</div> </div>     |
| 1   | CA    | 1539   | <div> <div>8%</div> <div>30% 55% 15%</div> </div>     |
| 2   | AB    | 218    | <div> <div>17%</div> <div>23% 51% 21% 5%</div> </div> |
| 2   | CB    | 218    | <div> <div>22%</div> <div>31% 49% 18% .</div> </div>  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 3   | AC    | 206    |                  |
| 3   | CC    | 206    |                  |
| 4   | AD    | 205    |                  |
| 4   | CD    | 205    |                  |
| 5   | AE    | 150    |                  |
| 5   | CE    | 150    |                  |
| 6   | AF    | 100    |                  |
| 6   | CF    | 100    |                  |
| 7   | AG    | 151    |                  |
| 7   | CG    | 151    |                  |
| 8   | AH    | 129    |                  |
| 8   | CH    | 129    |                  |
| 9   | AI    | 127    |                  |
| 9   | CI    | 127    |                  |
| 10  | AJ    | 98     |                  |
| 10  | CJ    | 98     |                  |
| 11  | AK    | 117    |                  |
| 11  | CK    | 117    |                  |
| 12  | AL    | 123    |                  |
| 12  | CL    | 123    |                  |
| 13  | AM    | 114    |                  |
| 13  | CM    | 114    |                  |
| 14  | AN    | 100    |                  |
| 14  | CN    | 100    |                  |
| 15  | AO    | 88     |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 15  | CO    | 88     |                  |
| 16  | AP    | 82     |                  |
| 16  | CP    | 82     |                  |
| 17  | AQ    | 80     |                  |
| 17  | CQ    | 80     |                  |
| 18  | AR    | 55     |                  |
| 18  | CR    | 55     |                  |
| 19  | AS    | 79     |                  |
| 19  | CS    | 79     |                  |
| 20  | AT    | 85     |                  |
| 20  | CT    | 85     |                  |
| 21  | AU    | 51     |                  |
| 21  | CU    | 51     |                  |
| 22  | BA    | 2903   |                  |
| 22  | DA    | 2903   |                  |
| 23  | BB    | 119    |                  |
| 23  | DB    | 119    |                  |
| 24  | BC    | 271    |                  |
| 24  | DC    | 271    |                  |
| 25  | BD    | 209    |                  |
| 25  | DD    | 209    |                  |
| 26  | BE    | 201    |                  |
| 26  | DE    | 201    |                  |
| 27  | BF    | 177    |                  |
| 27  | DF    | 177    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 28  | BG    | 176    |                  |
| 28  | DG    | 176    |                  |
| 29  | BH    | 149    |                  |
| 29  | DH    | 149    |                  |
| 30  | BI    | 141    |                  |
| 30  | DI    | 141    |                  |
| 31  | BJ    | 142    |                  |
| 31  | DJ    | 142    |                  |
| 32  | BK    | 122    |                  |
| 32  | DK    | 122    |                  |
| 33  | BL    | 143    |                  |
| 33  | DL    | 143    |                  |
| 34  | BM    | 136    |                  |
| 34  | DM    | 136    |                  |
| 35  | BN    | 120    |                  |
| 35  | DN    | 120    |                  |
| 36  | BO    | 116    |                  |
| 36  | DO    | 116    |                  |
| 37  | BP    | 114    |                  |
| 37  | DP    | 114    |                  |
| 38  | BQ    | 117    |                  |
| 38  | DQ    | 117    |                  |
| 39  | BR    | 103    |                  |
| 39  | DR    | 103    |                  |
| 40  | BS    | 110    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 40  | DS    | 110    |                  |
| 41  | BT    | 93     |                  |
| 41  | DT    | 93     |                  |
| 42  | BU    | 102    |                  |
| 42  | DU    | 102    |                  |
| 43  | BV    | 94     |                  |
| 43  | DV    | 94     |                  |
| 44  | BW    | 76     |                  |
| 44  | DW    | 76     |                  |
| 45  | BX    | 77     |                  |
| 45  | DX    | 77     |                  |
| 46  | BY    | 63     |                  |
| 46  | DY    | 63     |                  |
| 47  | BZ    | 58     |                  |
| 47  | DZ    | 58     |                  |
| 48  | B0    | 56     |                  |
| 48  | D0    | 56     |                  |
| 49  | B1    | 50     |                  |
| 49  | D1    | 50     |                  |
| 50  | B2    | 46     |                  |
| 50  | D2    | 46     |                  |
| 51  | B3    | 64     |                  |
| 51  | D3    | 64     |                  |
| 52  | B4    | 38     |                  |
| 52  | D4    | 38     |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 53  | B5    | 228    |                  |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 54  | MG   | AA    | 1656 | -         | -        | -       | X                |
| 54  | MG   | AA    | 1658 | -         | -        | -       | X                |
| 54  | MG   | AA    | 1662 | -         | -        | -       | X                |
| 54  | MG   | AA    | 1664 | -         | -        | -       | X                |
| 54  | MG   | AA    | 1668 | -         | -        | -       | X                |
| 54  | MG   | DA    | 3003 | -         | -        | -       | X                |
| 54  | MG   | DA    | 3005 | -         | -        | -       | X                |
| 54  | MG   | DA    | 3026 | -         | -        | -       | X                |
| 54  | MG   | DA    | 3028 | -         | -        | -       | X                |
| 54  | MG   | DA    | 3041 | -         | -        | -       | X                |
| 54  | MG   | DA    | 3044 | -         | -        | -       | X                |
| 54  | MG   | DA    | 3061 | -         | -        | -       | X                |
| 54  | MG   | DA    | 3062 | -         | -        | -       | X                |
| 54  | MG   | DA    | 3092 | -         | -        | -       | X                |
| 54  | MG   | DA    | 3100 | -         | -        | -       | X                |
| 54  | MG   | DA    | 3113 | -         | -        | -       | X                |
| 54  | MG   | DA    | 3119 | -         | -        | -       | X                |
| 54  | MG   | DA    | 3133 | -         | -        | -       | X                |
| 54  | MG   | DA    | 3135 | -         | -        | -       | X                |
| 54  | MG   | DA    | 3137 | -         | -        | -       | X                |
| 54  | MG   | DA    | 3151 | -         | -        | -       | X                |
| 54  | MG   | DA    | 3162 | -         | -        | -       | X                |
| 54  | MG   | DL    | 201  | -         | -        | -       | X                |
| 55  | DOL  | DA    | 3001 | -         | -        | X       | -                |

## 2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 288276 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

| Mol | Chain | Residues | Atoms |       |      |       |      | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|------|-------|------|---------|---------|-------|
| 1   | AA    | 1538     | Total | C     | N    | O     | P    | 0       | 0       | 0     |
|     |       |          | 32995 | 14716 | 6050 | 10691 | 1538 |         |         |       |
| 1   | CA    | 1539     | Total | C     | N    | O     | P    | 0       | 0       | 0     |
|     |       |          | 33015 | 14725 | 6052 | 10699 | 1539 |         |         |       |

- Molecule 2 is a protein called 30S ribosomal protein S2.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2   | AB    | 218      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1705  | 1081 | 305 | 312 | 7 |         |         |       |
| 2   | CB    | 218      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1705  | 1081 | 305 | 312 | 7 |         |         |       |

- Molecule 3 is a protein called 30S ribosomal protein S3.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 3   | AC    | 206      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1625  | 1028 | 305 | 289 | 3 |         |         |       |
| 3   | CC    | 206      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1625  | 1028 | 305 | 289 | 3 |         |         |       |

- Molecule 4 is a protein called 30S ribosomal protein S4.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 4   | AD    | 205      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1643  | 1026 | 315 | 298 | 4 |         |         |       |
| 4   | CD    | 205      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1643  | 1026 | 315 | 298 | 4 |         |         |       |

- Molecule 5 is a protein called 30S ribosomal protein S5.



| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 5   | AE    | 150      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1106  | 687 | 211 | 202 | 6 |         |         |       |
| 5   | CE    | 150      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1106  | 687 | 211 | 202 | 6 |         |         |       |

- Molecule 6 is a protein called 30S ribosomal protein S6.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 6   | AF    | 100      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 818   | 515 | 148 | 149 | 6 |         |         |       |
| 6   | CF    | 100      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 818   | 515 | 148 | 149 | 6 |         |         |       |

- Molecule 7 is a protein called 30S ribosomal protein S7.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 7   | AG    | 151      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1182  | 735 | 227 | 216 | 4 |         |         |       |
| 7   | CG    | 151      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1182  | 735 | 227 | 216 | 4 |         |         |       |

- Molecule 8 is a protein called 30S ribosomal protein S8.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 8   | AH    | 129      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 979   | 616 | 173 | 184 | 6 |         |         |       |
| 8   | CH    | 129      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 979   | 616 | 173 | 184 | 6 |         |         |       |

- Molecule 9 is a protein called 30S ribosomal protein S9.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 9   | AI    | 127      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1022  | 634 | 206 | 179 | 3 |         |         |       |
| 9   | CI    | 127      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1022  | 634 | 206 | 179 | 3 |         |         |       |

- Molecule 10 is a protein called 30S ribosomal protein S10.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10  | AJ    | 98       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 787   | 493 | 150 | 143 | 1 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 10  | CJ    | 98       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 787   | 493 | 150 | 143 | 1 |         |         |       |

- Molecule 11 is a protein called 30S ribosomal protein S11.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 11  | AK    | 117      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 877   | 540 | 174 | 160 | 3 |         |         |       |
| 11  | CK    | 117      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 877   | 540 | 174 | 160 | 3 |         |         |       |

- Molecule 12 is a protein called 30S ribosomal protein S12.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 12  | AL    | 123      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 955   | 590 | 196 | 165 | 4 |         |         |       |
| 12  | CL    | 123      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 955   | 590 | 196 | 165 | 4 |         |         |       |

- Molecule 13 is a protein called 30S ribosomal protein S13.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 13  | AM    | 114      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 884   | 546 | 178 | 157 | 3 |         |         |       |
| 13  | CM    | 114      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 884   | 546 | 178 | 157 | 3 |         |         |       |

- Molecule 14 is a protein called 30S ribosomal protein S14.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 14  | AN    | 96       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 774   | 483 | 160 | 128 | 3 |         |         |       |
| 14  | CN    | 96       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 774   | 483 | 160 | 128 | 3 |         |         |       |

- Molecule 15 is a protein called 30S ribosomal protein S15.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 15  | AO    | 88       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 710   | 437 | 143 | 129 | 1 |         |         |       |
| 15  | CO    | 88       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 710   | 437 | 143 | 129 | 1 |         |         |       |

- Molecule 16 is a protein called 30S ribosomal protein S16.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 16  | AP    | 82       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 649   | 406 | 128 | 114 | 1 |         |         |       |
| 16  | CP    | 82       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 649   | 406 | 128 | 114 | 1 |         |         |       |

- Molecule 17 is a protein called 30S ribosomal protein S17.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 17  | AQ    | 80       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 649   | 411 | 121 | 114 | 3 |         |         |       |
| 17  | CQ    | 80       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 649   | 411 | 121 | 114 | 3 |         |         |       |

- Molecule 18 is a protein called 30S ribosomal protein S18.

| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 18  | AR    | 55       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 456   | 288 | 86 | 82 |         |         |       |
| 18  | CR    | 55       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 456   | 288 | 86 | 82 |         |         |       |

- Molecule 19 is a protein called 30S ribosomal protein S19.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 19  | AS    | 79       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 638   | 408 | 120 | 108 | 2 |         |         |       |
| 19  | CS    | 79       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 638   | 408 | 120 | 108 | 2 |         |         |       |

- Molecule 20 is a protein called 30S ribosomal protein S20.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 20  | AT    | 85       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 665   | 411 | 137 | 114 | 3 |         |         |       |
| 20  | CT    | 85       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 665   | 411 | 137 | 114 | 3 |         |         |       |

- Molecule 21 is a protein called 30S ribosomal protein S21.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 21  | AU    | 51       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 426   | 265 | 86 | 74 | 1 |         |         |       |
| 21  | CU    | 51       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 426   | 265 | 86 | 74 | 1 |         |         |       |

- Molecule 22 is a RNA chain called 23S rRNA.

| Mol | Chain | Residues | Atoms |       |       |       |      | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-------|-------|-------|------|---------|---------|-------|
| 22  | BA    | 2897     | Total | C     | N     | O     | P    | 0       | 0       | 0     |
|     |       |          | 62195 | 27745 | 11446 | 20107 | 2897 |         |         |       |
| 22  | DA    | 2897     | Total | C     | N     | O     | P    | 0       | 0       | 0     |
|     |       |          | 62195 | 27745 | 11446 | 20107 | 2897 |         |         |       |

- Molecule 23 is a RNA chain called 5S rRNA.

| Mol | Chain | Residues | Atoms |      |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|-----|---------|---------|-------|
| 23  | BB    | 119      | Total | C    | N   | O   | P   | 0       | 0       | 0     |
|     |       |          | 2549  | 1135 | 466 | 829 | 119 |         |         |       |
| 23  | DB    | 118      | Total | C    | N   | O   | P   | 0       | 0       | 0     |
|     |       |          | 2529  | 1126 | 464 | 821 | 118 |         |         |       |

- Molecule 24 is a protein called 50S ribosomal protein L2.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 24  | BC    | 271      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2083  | 1288 | 423 | 365 | 7 |         |         |       |
| 24  | DC    | 271      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2083  | 1288 | 423 | 365 | 7 |         |         |       |

- Molecule 25 is a protein called 50S ribosomal protein L3.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 25  | BD    | 209      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1565  | 979 | 288 | 294 | 4 |         |         |       |
| 25  | DD    | 209      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1565  | 979 | 288 | 294 | 4 |         |         |       |

- Molecule 26 is a protein called 50S ribosomal protein L4.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 26  | BE    | 201      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1552  | 974 | 283 | 290 | 5 |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 26  | DE    | 201      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1552  | 974 | 283 | 290 | 5 |         |         |       |

- Molecule 27 is a protein called 50S ribosomal protein L5.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 27  | BF    | 177      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1411  | 899 | 249 | 257 | 6 |         |         |       |
| 27  | DF    | 177      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1411  | 899 | 249 | 257 | 6 |         |         |       |

- Molecule 28 is a protein called 50S ribosomal protein L6.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 28  | BG    | 176      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1323  | 832 | 243 | 246 | 2 |         |         |       |
| 28  | DG    | 176      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1323  | 832 | 243 | 246 | 2 |         |         |       |

- Molecule 29 is a protein called 50S ribosomal protein L9.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 29  | BH    | 149      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1110  | 699 | 197 | 213 | 1 |         |         |       |
| 29  | DH    | 149      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1110  | 699 | 197 | 213 | 1 |         |         |       |

- Molecule 30 is a protein called 50S ribosomal protein L11.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 30  | BI    | 141      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1032  | 651 | 179 | 196 | 6 |         |         |       |
| 30  | DI    | 141      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1032  | 651 | 179 | 196 | 6 |         |         |       |

- Molecule 31 is a protein called 50S ribosomal protein L13.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 31  | BJ    | 142      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1129  | 714 | 212 | 199 | 4 |         |         |       |
| 31  | DJ    | 142      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1129  | 714 | 212 | 199 | 4 |         |         |       |

- Molecule 32 is a protein called 50S ribosomal protein L14.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 32  | BK    | 122      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 939   | 587 | 180 | 166 | 6 |         |         |       |
| 32  | DK    | 122      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 939   | 587 | 180 | 166 | 6 |         |         |       |

- Molecule 33 is a protein called 50S ribosomal protein L15.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 33  | BL    | 143      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1045  | 649 | 206 | 189 | 1 |         |         |       |
| 33  | DL    | 143      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1045  | 649 | 206 | 189 | 1 |         |         |       |

- Molecule 34 is a protein called 50S ribosomal protein L16.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 34  | BM    | 136      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1074  | 686 | 205 | 177 | 6 |         |         |       |
| 34  | DM    | 136      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1074  | 686 | 205 | 177 | 6 |         |         |       |

- Molecule 35 is a protein called 50S ribosomal protein L17.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 35  | BN    | 120      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 961   | 593 | 196 | 167 | 5 |         |         |       |
| 35  | DN    | 120      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 961   | 593 | 196 | 167 | 5 |         |         |       |

- Molecule 36 is a protein called 50S ribosomal protein L18.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 36  | BO    | 116      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 892   | 552 | 178 | 162 |         |         |       |
| 36  | DO    | 116      | Total | C   | N   | O   | 0       | 0       | 0     |
|     |       |          | 892   | 552 | 178 | 162 |         |         |       |

- Molecule 37 is a protein called 50S ribosomal protein L19.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 37  | BP    | 114      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 917   | 574 | 179 | 163 | 1 |         |         |       |
| 37  | DP    | 114      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 917   | 574 | 179 | 163 | 1 |         |         |       |

- Molecule 38 is a protein called 50S ribosomal protein L20.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 38  | BQ    | 117      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 947   | 604 | 192 | 151 |   |         |         |       |
| 38  | DQ    | 117      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 947   | 604 | 192 | 151 |   |         |         |       |

- Molecule 39 is a protein called 50S ribosomal protein L21.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 39  | BR    | 103      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 816   | 516 | 153 | 145 | 2 |         |         |       |
| 39  | DR    | 103      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 816   | 516 | 153 | 145 | 2 |         |         |       |

- Molecule 40 is a protein called 50S ribosomal protein L22.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 40  | BS    | 110      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 857   | 532 | 166 | 156 | 3 |         |         |       |
| 40  | DS    | 110      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 857   | 532 | 166 | 156 | 3 |         |         |       |

- Molecule 41 is a protein called 50S ribosomal protein L23.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 41  | BT    | 93       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 739   | 466 | 139 | 132 | 2 |         |         |       |
| 41  | DT    | 93       | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 739   | 466 | 139 | 132 | 2 |         |         |       |

- Molecule 42 is a protein called 50S ribosomal protein L24.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 42  | BU    | 102      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 780   | 492 | 146 | 142 |   |         |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 42  | DU    | 102      | Total | C   | N   | O   |         |         |       |
|     |       |          | 780   | 492 | 146 | 142 | 0       | 0       | 0     |

- Molecule 43 is a protein called 50S ribosomal protein L25.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 43  | BV    | 94       | Total | C   | N   | O   | S       |         |       |
|     |       |          | 753   | 479 | 137 | 134 | 3       | 0       | 0     |
| 43  | DV    | 94       | Total | C   | N   | O   | S       |         |       |
|     |       |          | 753   | 479 | 137 | 134 | 3       | 0       | 0     |

- Molecule 44 is a protein called 50S ribosomal protein L27.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 44  | BW    | 76       | Total | C   | N   | O   | S       |         |       |
|     |       |          | 580   | 359 | 117 | 103 | 1       | 0       | 0     |
| 44  | DW    | 75       | Total | C   | N   | O   | S       |         |       |
|     |       |          | 569   | 353 | 113 | 102 | 1       | 0       | 0     |

- Molecule 45 is a protein called 50S ribosomal protein L28.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 45  | BX    | 77       | Total | C   | N   | O   | S       |         |       |
|     |       |          | 625   | 388 | 129 | 106 | 2       | 0       | 0     |
| 45  | DX    | 77       | Total | C   | N   | O   | S       |         |       |
|     |       |          | 625   | 388 | 129 | 106 | 2       | 0       | 0     |

- Molecule 46 is a protein called 50S ribosomal protein L29.

| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 46  | BY    | 63       | Total | C   | N  | O  | S       |         |       |
|     |       |          | 509   | 313 | 99 | 95 | 2       | 0       | 0     |
| 46  | DY    | 63       | Total | C   | N  | O  | S       |         |       |
|     |       |          | 509   | 313 | 99 | 95 | 2       | 0       | 0     |

- Molecule 47 is a protein called 50S ribosomal protein L30.

| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 47  | BZ    | 58       | Total | C   | N  | O  | S       |         |       |
|     |       |          | 449   | 281 | 87 | 79 | 2       | 0       | 0     |
| 47  | DZ    | 58       | Total | C   | N  | O  | S       |         |       |
|     |       |          | 449   | 281 | 87 | 79 | 2       | 0       | 0     |



- Molecule 48 is a protein called 50S ribosomal protein L32.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 48  | B0    | 56       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 444   | 269 | 94 | 80 | 1 |         |         |       |
| 48  | D0    | 56       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 444   | 269 | 94 | 80 | 1 |         |         |       |

- Molecule 49 is a protein called 50S ribosomal protein L33.

| Mol | Chain | Residues | Atoms |     |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 49  | B1    | 50       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 410   | 263 | 75 | 72 |         |         |       |
| 49  | D1    | 50       | Total | C   | N  | O  | 0       | 0       | 0     |
|     |       |          | 410   | 263 | 75 | 72 |         |         |       |

- Molecule 50 is a protein called 50S ribosomal protein L34.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 50  | B2    | 46       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 377   | 228 | 90 | 57 | 2 |         |         |       |
| 50  | D2    | 46       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 377   | 228 | 90 | 57 | 2 |         |         |       |

- Molecule 51 is a protein called 50S ribosomal protein L35.

| Mol | Chain | Residues | Atoms |     |     |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|----|---|---------|---------|-------|
| 51  | B3    | 64       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 504   | 323 | 105 | 74 | 2 |         |         |       |
| 51  | D3    | 64       | Total | C   | N   | O  | S | 0       | 0       | 0     |
|     |       |          | 504   | 323 | 105 | 74 | 2 |         |         |       |

- Molecule 52 is a protein called 50S ribosomal protein L36.

| Mol | Chain | Residues | Atoms |     |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 52  | B4    | 38       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 302   | 185 | 65 | 48 | 4 |         |         |       |
| 52  | D4    | 38       | Total | C   | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 302   | 185 | 65 | 48 | 4 |         |         |       |

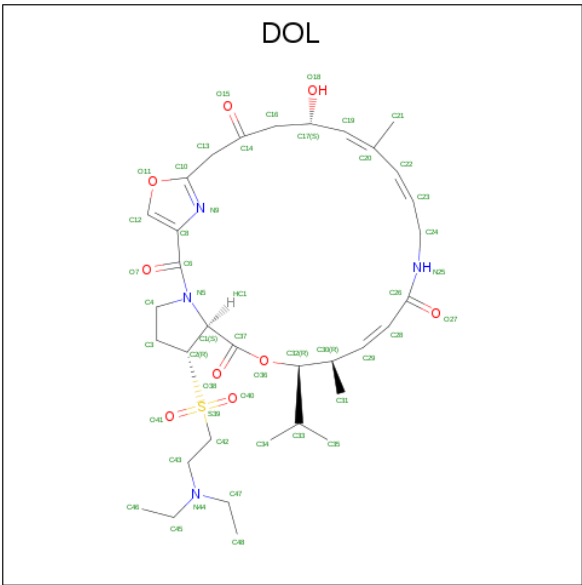
- Molecule 53 is a protein called 50S ribosomal protein L1.

| Mol | Chain | Residues | Atoms |     |     |     | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|---------|-------|
| 53  | B5    | 191      | Total | C   | N   | O   | 0       | 0       | 1     |
|     |       |          | 1142  | 691 | 221 | 230 |         |         |       |

- Molecule 54 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 54  | BB    | 4        | Total | Mg  | 0       | 0       |
|     |       |          | 4     | 4   |         |         |
| 54  | BA    | 194      | Total | Mg  | 0       | 0       |
|     |       |          | 194   | 194 |         |         |
| 54  | CA    | 56       | Total | Mg  | 0       | 0       |
|     |       |          | 56    | 56  |         |         |
| 54  | DQ    | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 54  | DL    | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 54  | D2    | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 54  | DA    | 164      | Total | Mg  | 0       | 0       |
|     |       |          | 164   | 164 |         |         |
| 54  | AA    | 70       | Total | Mg  | 0       | 0       |
|     |       |          | 70    | 70  |         |         |
| 54  | BQ    | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 54  | AN    | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 54  | DB    | 3        | Total | Mg  | 0       | 0       |
|     |       |          | 3     | 3   |         |         |
| 54  | AM    | 1        | Total | Mg  | 0       | 0       |
|     |       |          | 1     | 1   |         |         |

- Molecule 55 is 5-(2-DIETHYLAMINO-ETHANESULFONYL)-21-HYDROXY-10-ISOPROPYL-11,19-DIMETHYL-9,26-DIOXA-3,15,28-TRIAZA-TRICYCLO[23.2.1.00,255]OCTACOSA-1(27),12,17,19,25(28)-PENTAENE-2,8,14,23-TETRAONE (three-letter code: DOL) (formula: C<sub>34</sub>H<sub>50</sub>N<sub>4</sub>O<sub>9</sub>S).



| Mol | Chain | Residues | Atoms |    |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|---------|
| 55  | BA    | 1        | Total | C  | N | O | S | 0       | 0       |
|     |       |          | 48    | 34 | 4 | 9 | 1 |         |         |
| 55  | DA    | 1        | Total | C  | N | O | S | 0       | 0       |
|     |       |          | 48    | 34 | 4 | 9 | 1 |         |         |

- Molecule 56 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 56  | B4    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |
| 56  | D4    | 1        | Total | Zn | 0       | 0       |
|     |       |          | 1     | 1  |         |         |

- Molecule 57 is water.

| Mol | Chain | Residues | Atoms |     | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 57  | AA    | 195      | Total | O   | 0       | 0       |
|     |       |          | 195   | 195 |         |         |
| 57  | AE    | 1        | Total | O   | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 57  | AL    | 1        | Total | O   | 0       | 0       |
|     |       |          | 1     | 1   |         |         |
| 57  | AN    | 3        | Total | O   | 0       | 0       |
|     |       |          | 3     | 3   |         |         |
| 57  | AT    | 2        | Total | O   | 0       | 0       |
|     |       |          | 2     | 2   |         |         |

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| Mol | Chain | Residues | Atoms              | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 57  | AU    | 1        | Total O<br>1 1     | 0       | 0       |
| 57  | BA    | 615      | Total O<br>615 615 | 0       | 0       |
| 57  | BB    | 13       | Total O<br>13 13   | 0       | 0       |
| 57  | BC    | 8        | Total O<br>8 8     | 0       | 0       |
| 57  | BD    | 3        | Total O<br>3 3     | 0       | 0       |
| 57  | BE    | 2        | Total O<br>2 2     | 0       | 0       |
| 57  | BF    | 1        | Total O<br>1 1     | 0       | 0       |
| 57  | BL    | 7        | Total O<br>7 7     | 0       | 0       |
| 57  | BN    | 5        | Total O<br>5 5     | 0       | 0       |
| 57  | BQ    | 1        | Total O<br>1 1     | 0       | 0       |
| 57  | BS    | 1        | Total O<br>1 1     | 0       | 0       |
| 57  | BT    | 1        | Total O<br>1 1     | 0       | 0       |
| 57  | BU    | 1        | Total O<br>1 1     | 0       | 0       |
| 57  | BV    | 1        | Total O<br>1 1     | 0       | 0       |
| 57  | B2    | 1        | Total O<br>1 1     | 0       | 0       |
| 57  | B3    | 3        | Total O<br>3 3     | 0       | 0       |
| 57  | B4    | 2        | Total O<br>2 2     | 0       | 0       |
| 57  | CA    | 193      | Total O<br>193 193 | 0       | 0       |
| 57  | CL    | 1        | Total O<br>1 1     | 0       | 0       |
| 57  | CN    | 1        | Total O<br>1 1     | 0       | 0       |
| 57  | CT    | 2        | Total O<br>2 2     | 0       | 0       |

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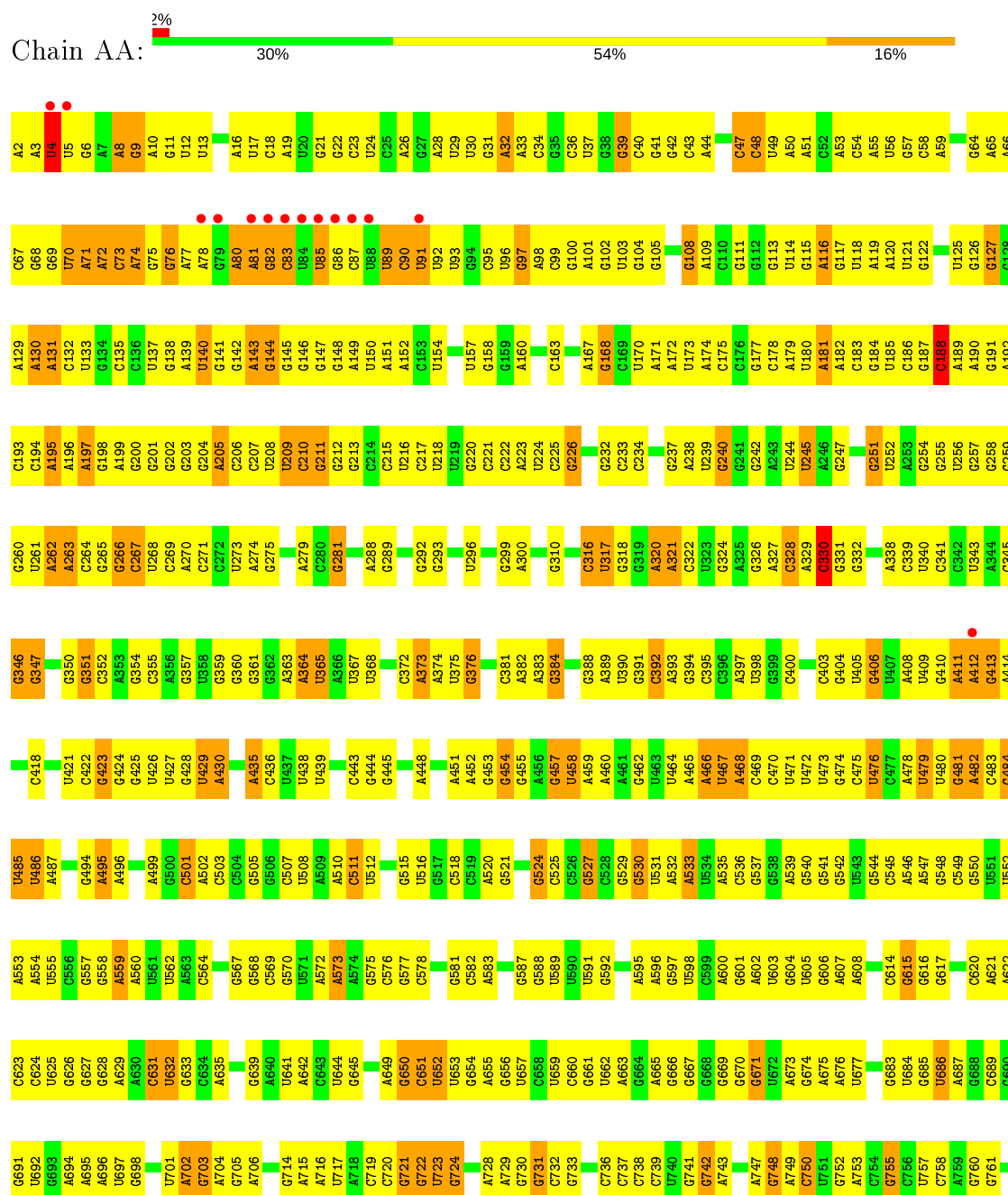
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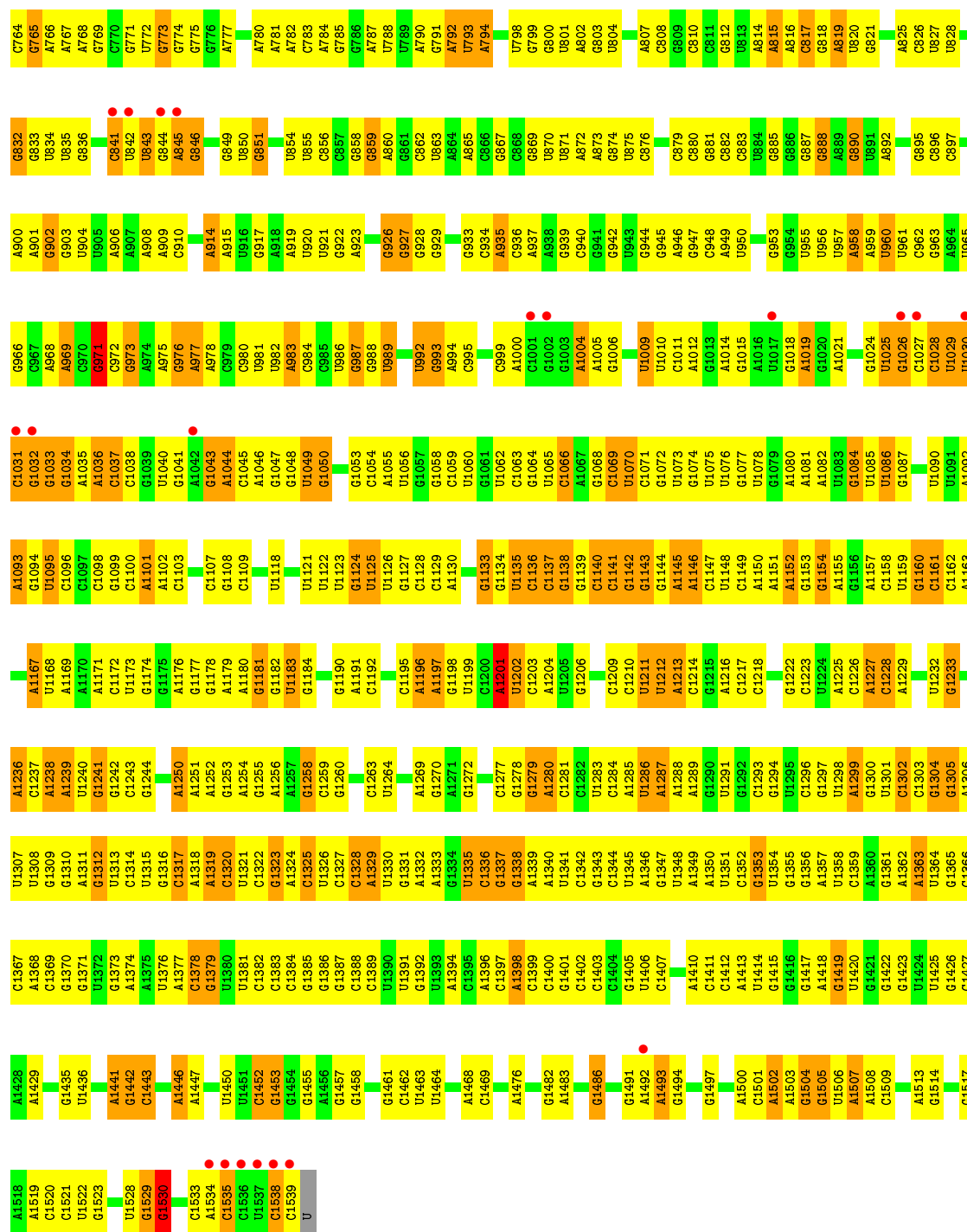
| Mol | Chain | Residues | Atoms        |          | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 57  | CU    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 57  | DA    | 608      | Total<br>608 | O<br>608 | 0       | 0       |
| 57  | DB    | 13       | Total<br>13  | O<br>13  | 0       | 0       |
| 57  | DC    | 10       | Total<br>10  | O<br>10  | 0       | 0       |
| 57  | DD    | 4        | Total<br>4   | O<br>4   | 0       | 0       |
| 57  | DE    | 4        | Total<br>4   | O<br>4   | 0       | 0       |
| 57  | DJ    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 57  | DL    | 4        | Total<br>4   | O<br>4   | 0       | 0       |
| 57  | DN    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 57  | DS    | 2        | Total<br>2   | O<br>2   | 0       | 0       |
| 57  | DT    | 3        | Total<br>3   | O<br>3   | 0       | 0       |
| 57  | DU    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 57  | DV    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 57  | D2    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 57  | D3    | 1        | Total<br>1   | O<br>1   | 0       | 0       |
| 57  | D4    | 1        | Total<br>1   | O<br>1   | 0       | 0       |

### 3 Residue-property plots

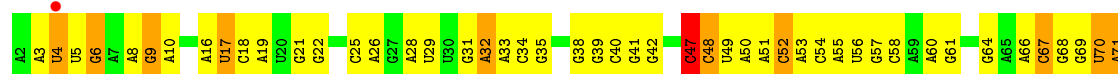
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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 dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: 16S rRNA



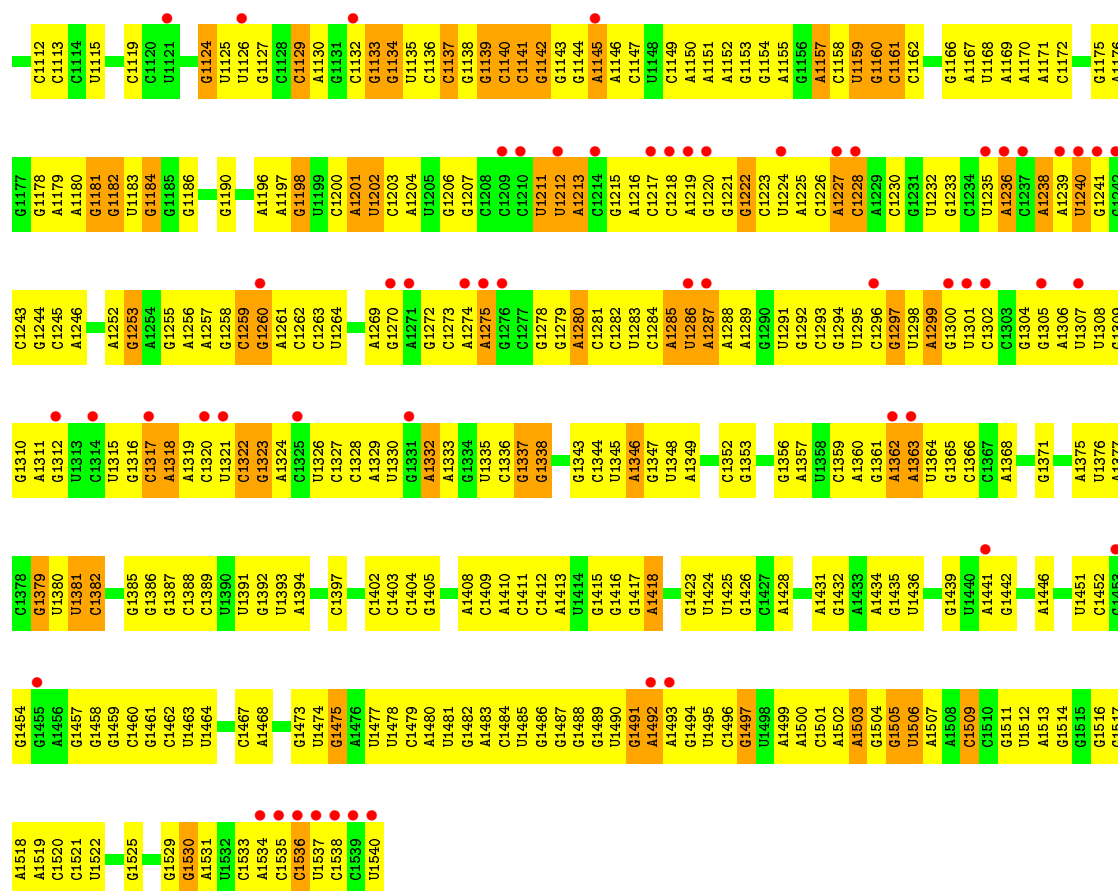


• Molecule 1: 16S rRNA

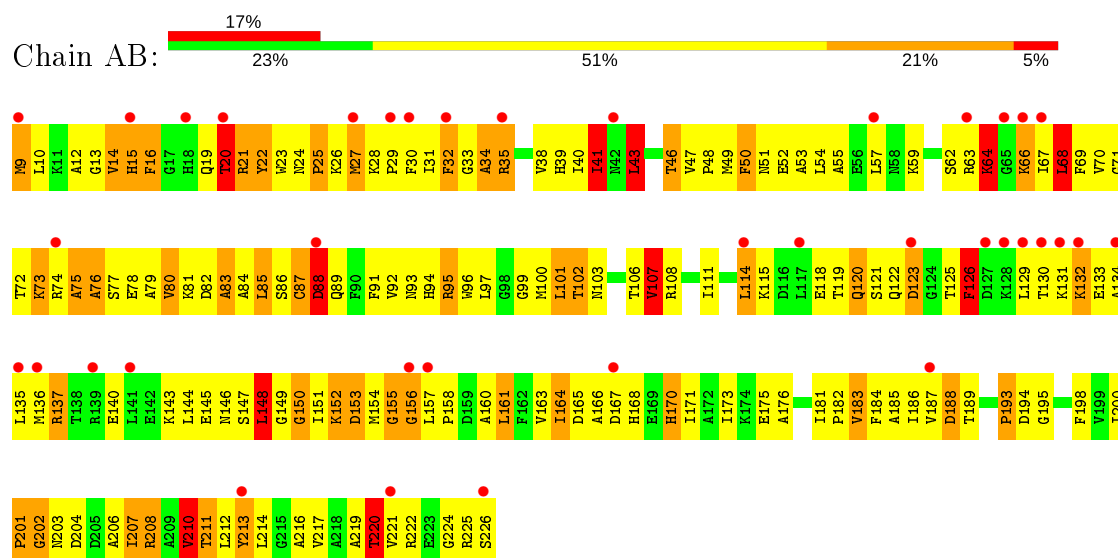






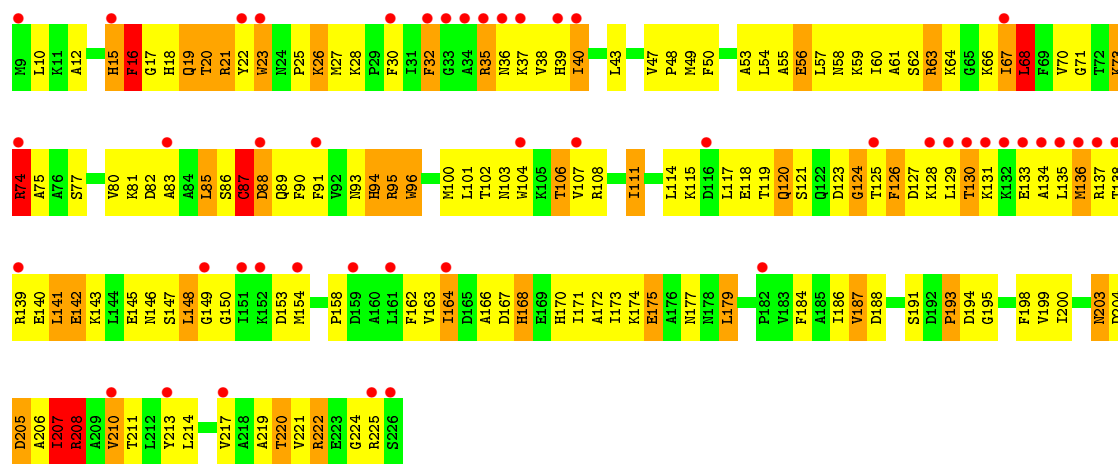


• Molecule 2: 30S ribosomal protein S2

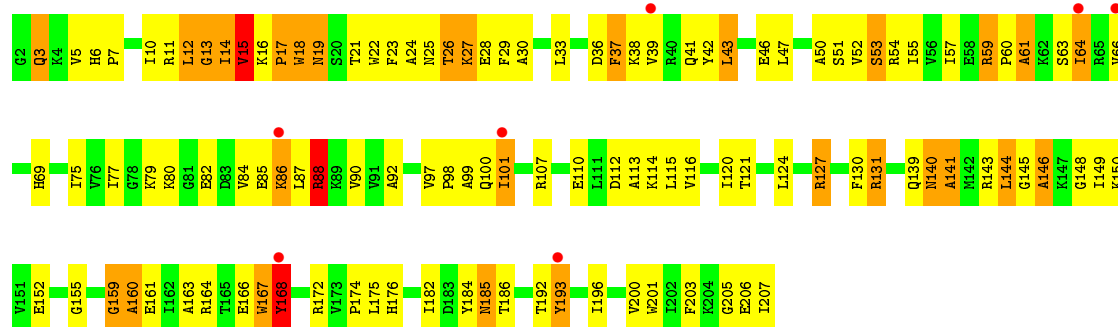


• Molecule 2: 30S ribosomal protein S2

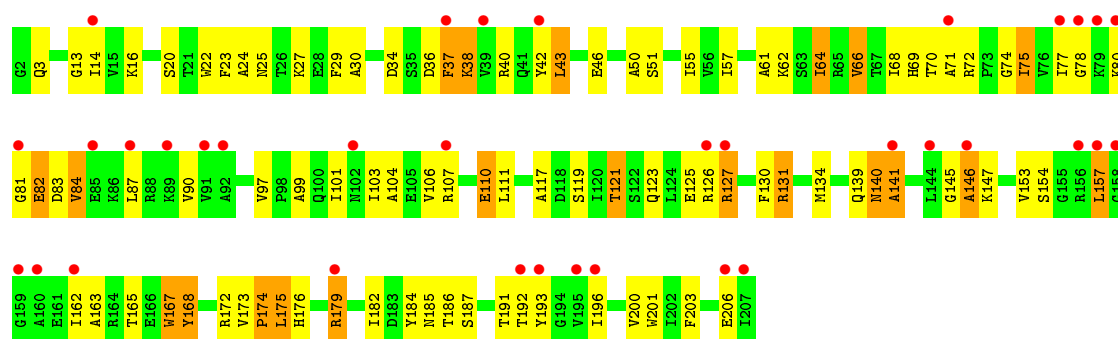




• Molecule 3: 30S ribosomal protein S3

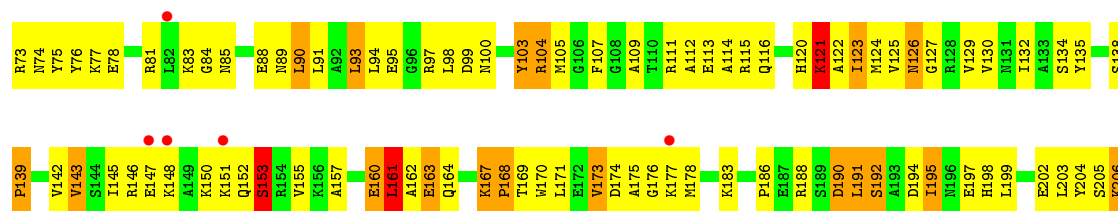


• Molecule 3: 30S ribosomal protein S3

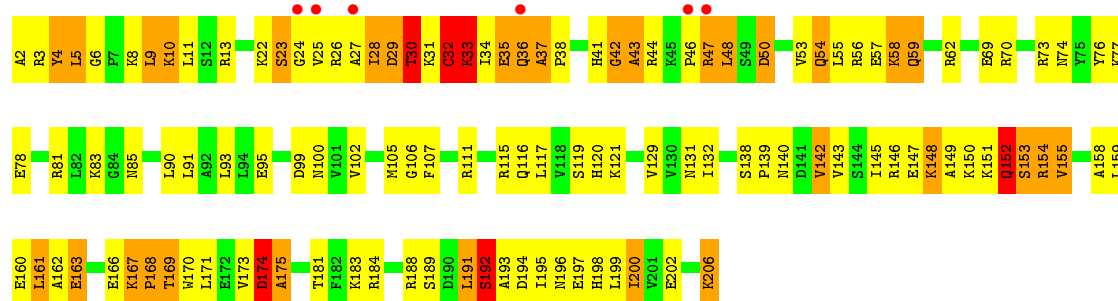
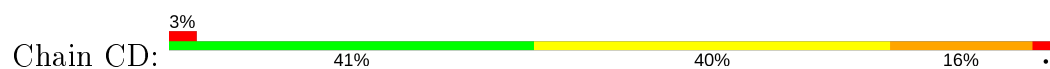


• Molecule 4: 30S ribosomal protein S4

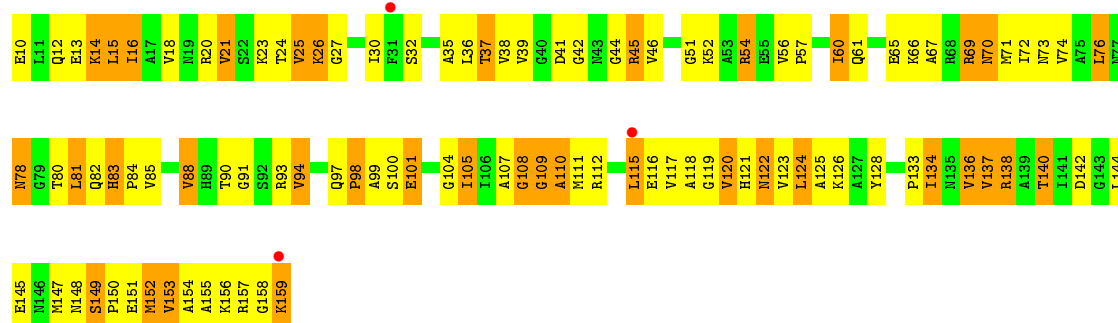




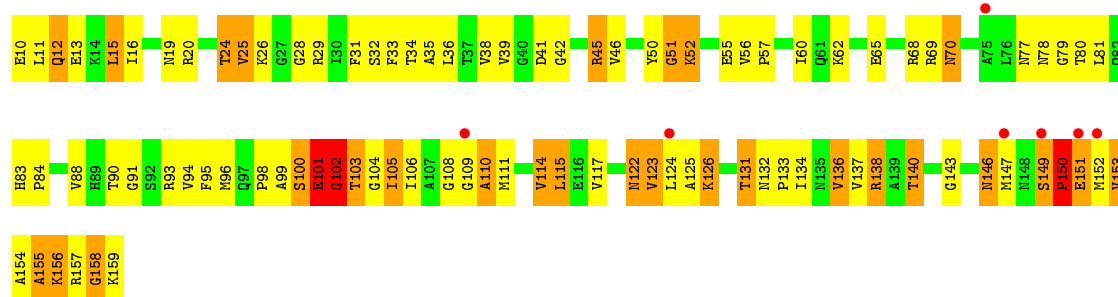
• Molecule 4: 30S ribosomal protein S4



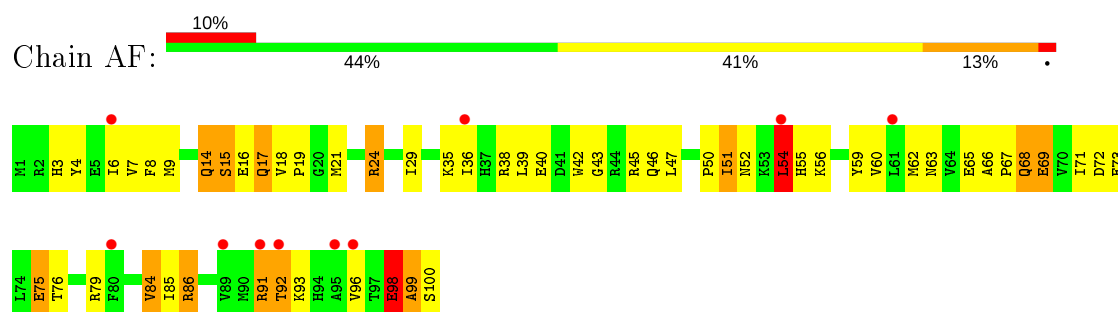
• Molecule 5: 30S ribosomal protein S5



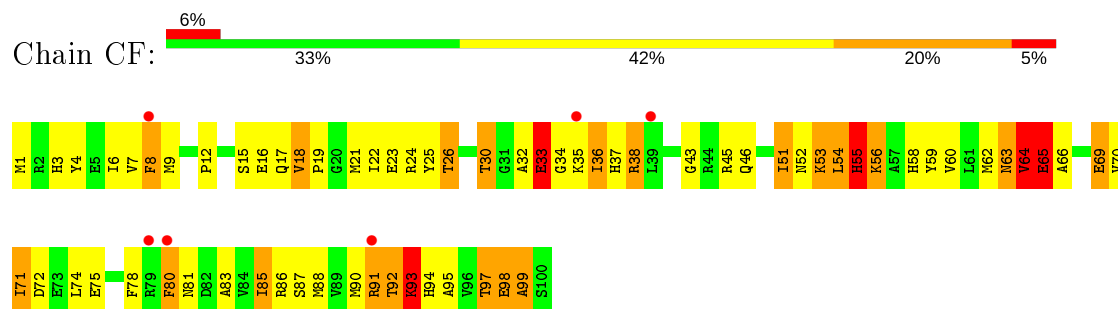
• Molecule 5: 30S ribosomal protein S5



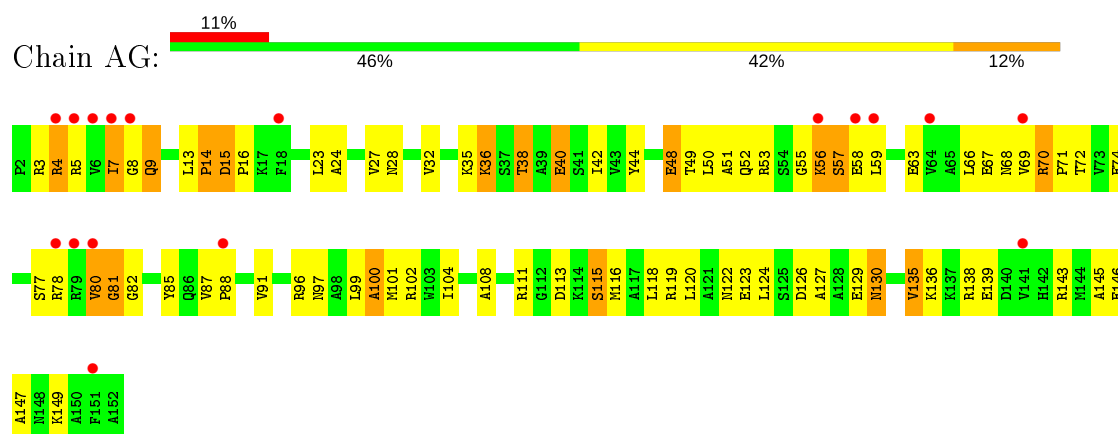
• Molecule 6: 30S ribosomal protein S6



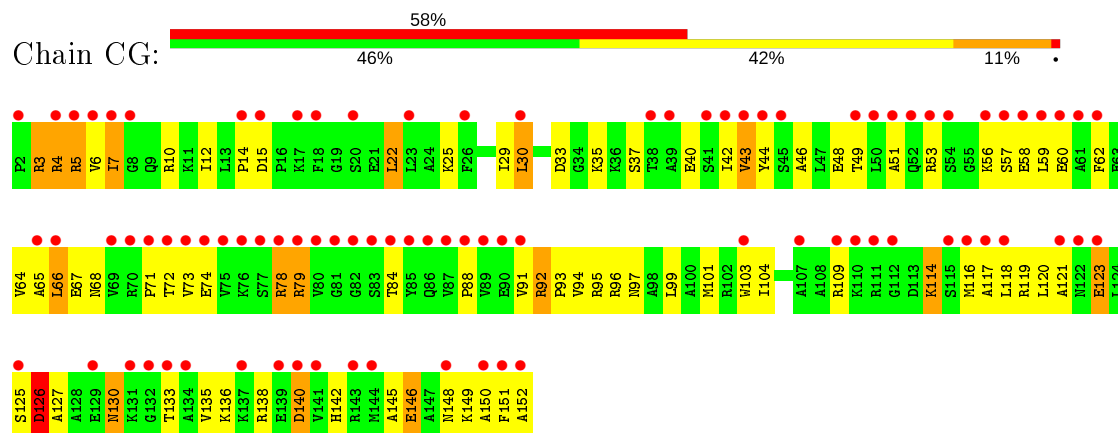
- Molecule 6: 30S ribosomal protein S6



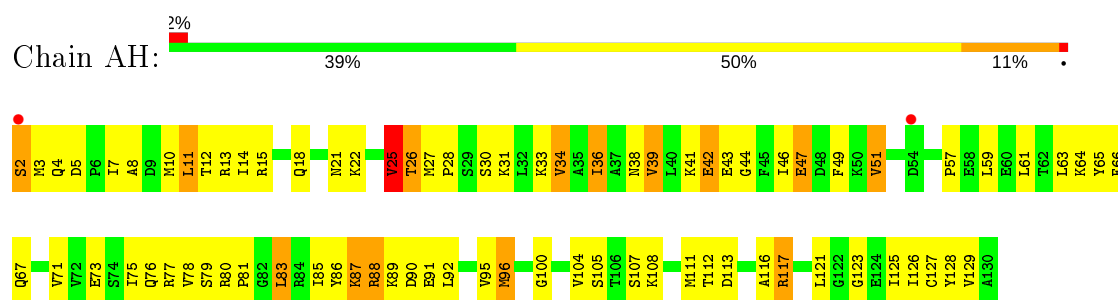
- Molecule 7: 30S ribosomal protein S7



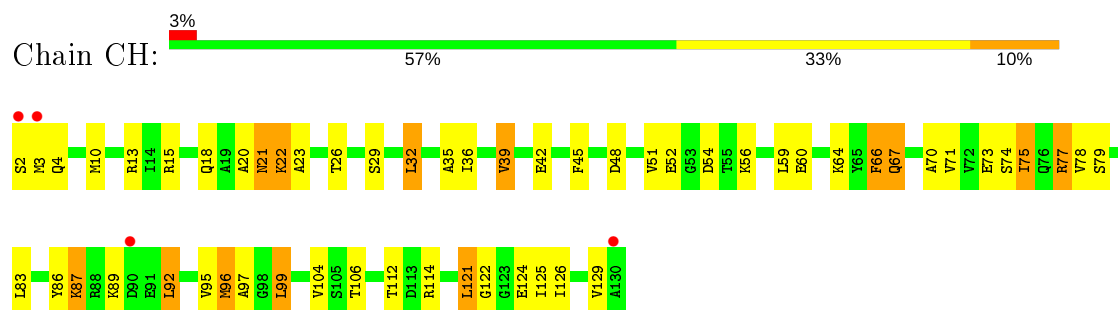
- Molecule 7: 30S ribosomal protein S7



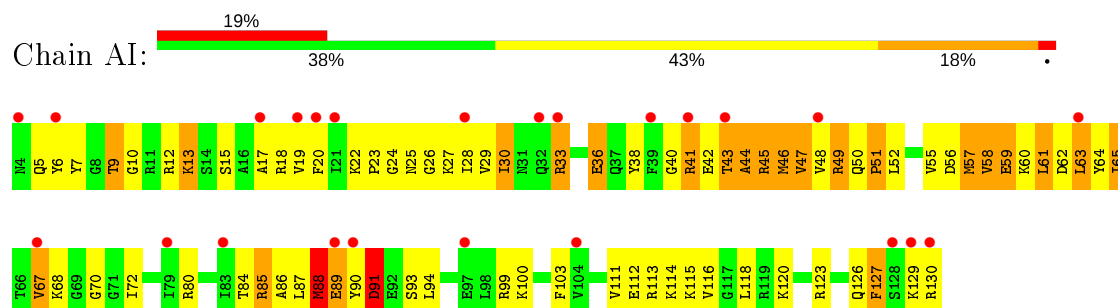
- Molecule 8: 30S ribosomal protein S8



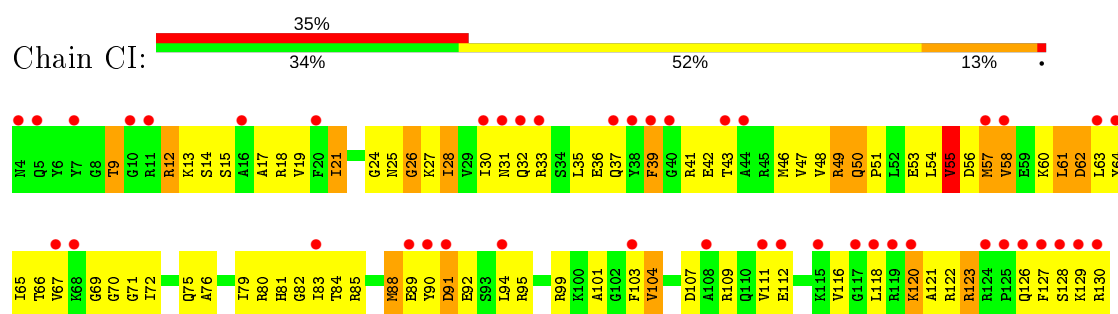
- Molecule 8: 30S ribosomal protein S8



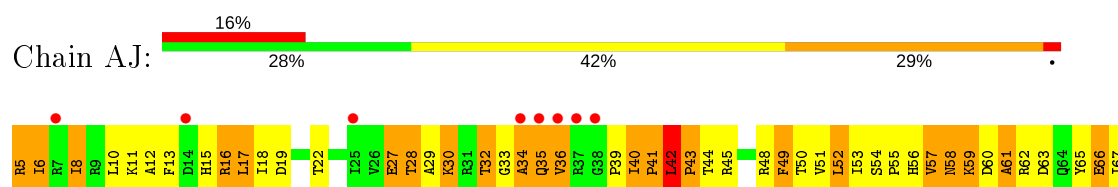
- Molecule 9: 30S ribosomal protein S9

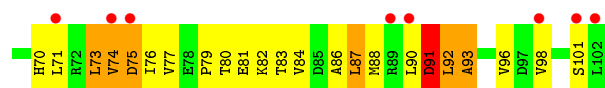


- Molecule 9: 30S ribosomal protein S9

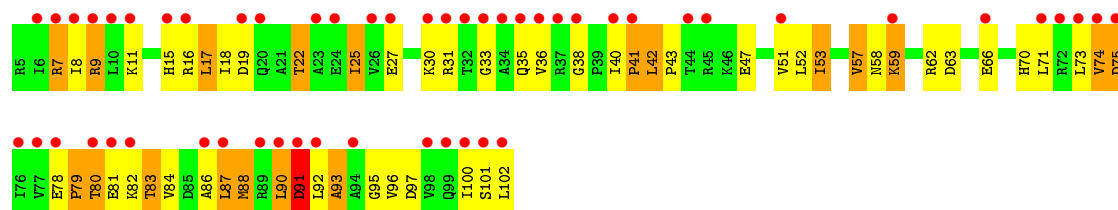
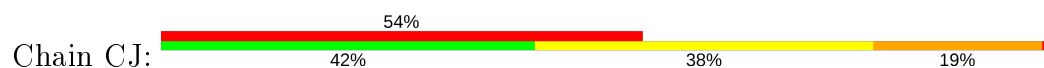


- Molecule 10: 30S ribosomal protein S10

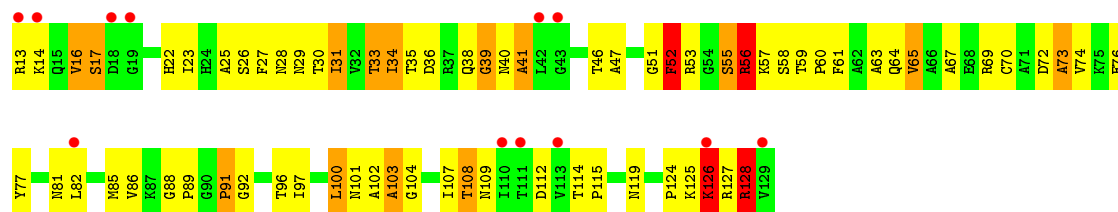
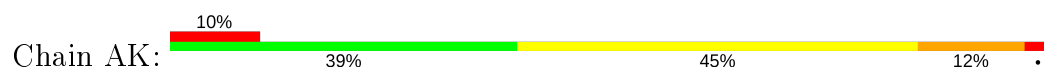




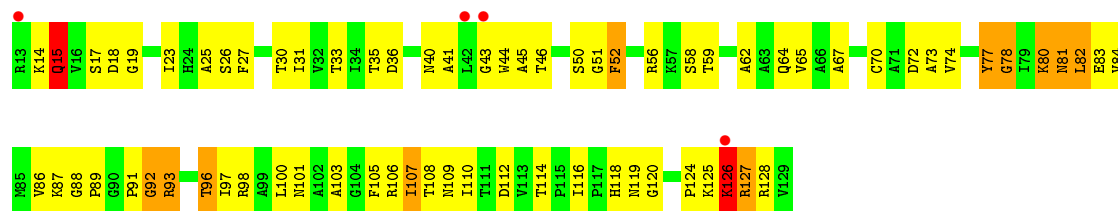
- Molecule 10: 30S ribosomal protein S10



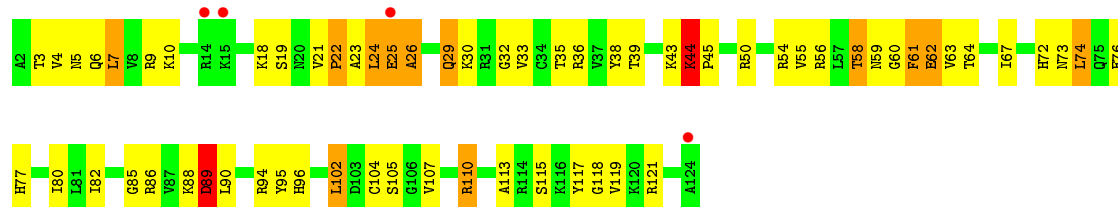
- Molecule 11: 30S ribosomal protein S11



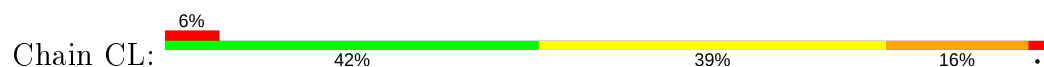
- Molecule 11: 30S ribosomal protein S11

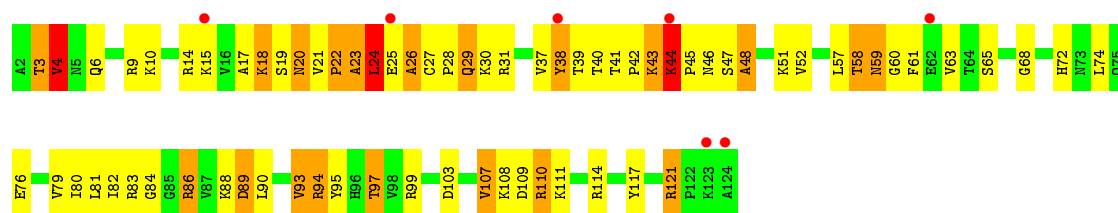


- Molecule 12: 30S ribosomal protein S12

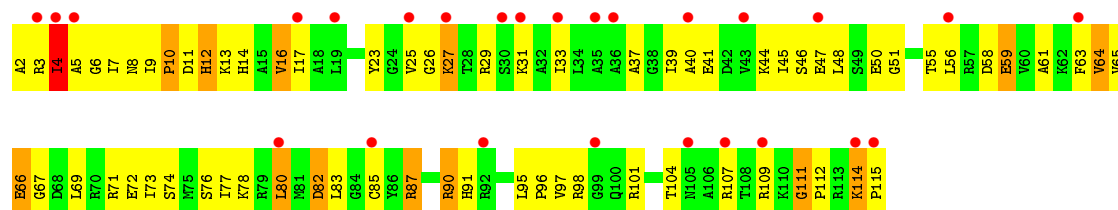


- Molecule 12: 30S ribosomal protein S12

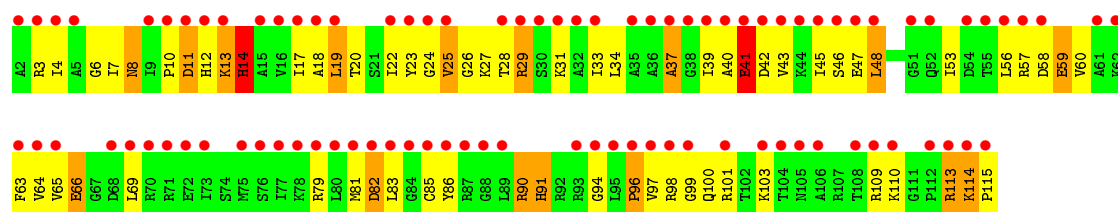
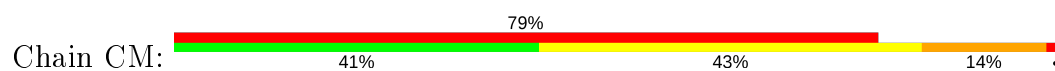




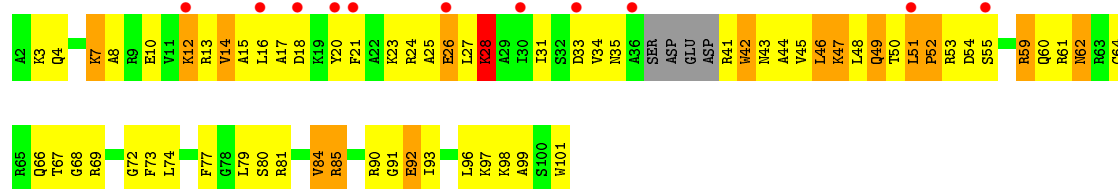
• Molecule 13: 30S ribosomal protein S13



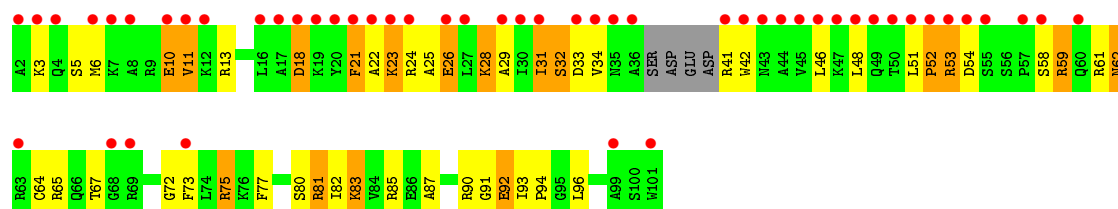
• Molecule 13: 30S ribosomal protein S13



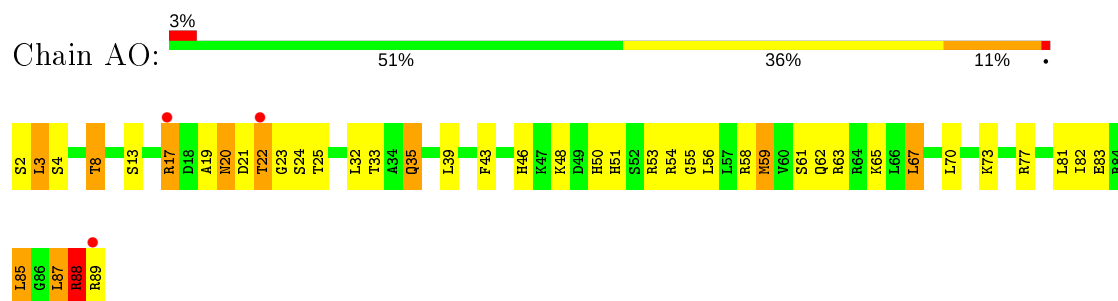
• Molecule 14: 30S ribosomal protein S14



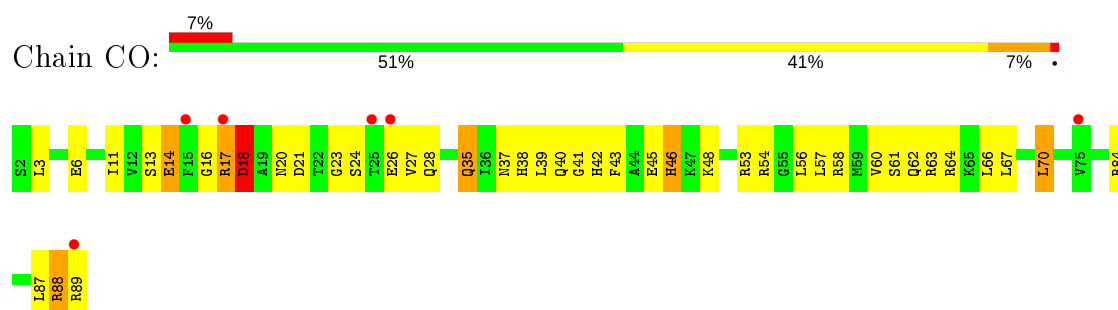
• Molecule 14: 30S ribosomal protein S14



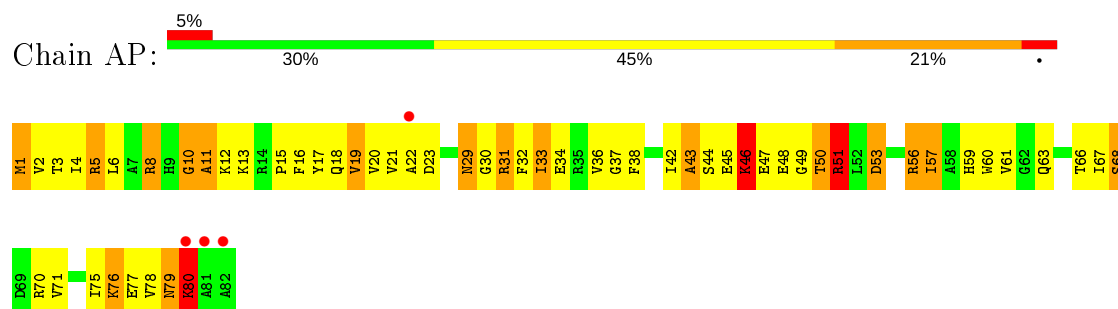
- Molecule 15: 30S ribosomal protein S15



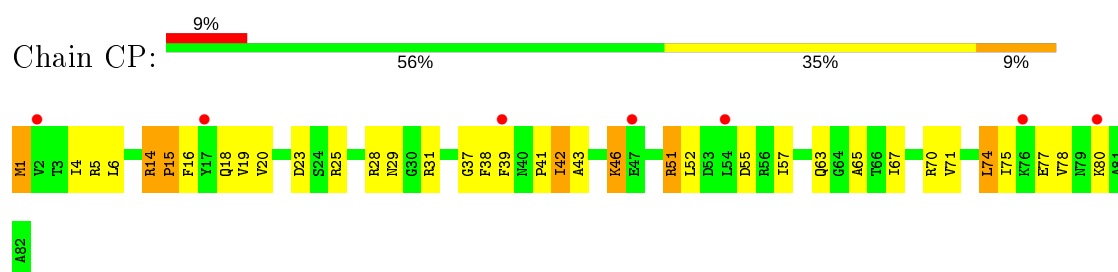
- Molecule 15: 30S ribosomal protein S15



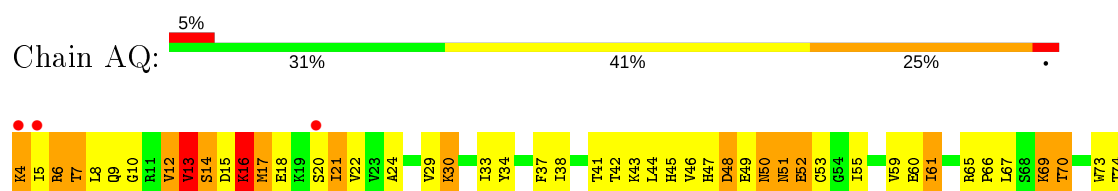
- Molecule 16: 30S ribosomal protein S16



- Molecule 16: 30S ribosomal protein S16



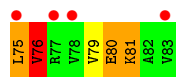
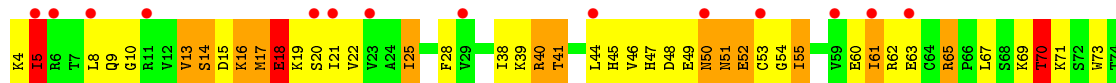
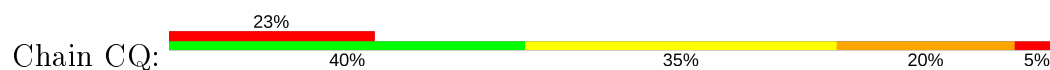
- Molecule 17: 30S ribosomal protein S17







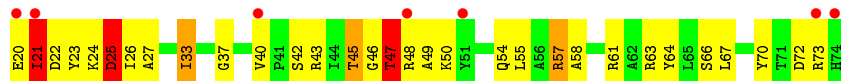
- Molecule 17: 30S ribosomal protein S17



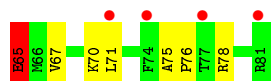
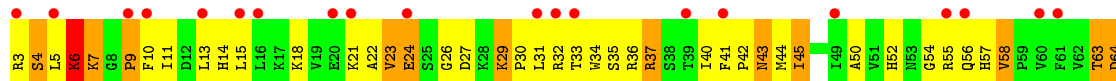
- Molecule 18: 30S ribosomal protein S18



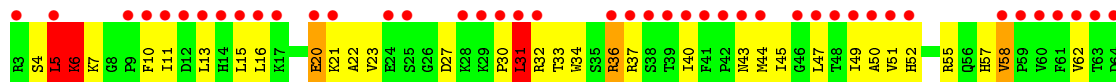
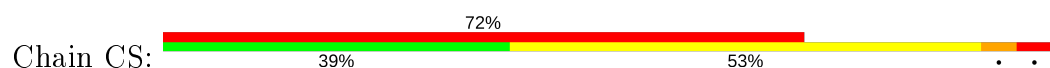
- Molecule 18: 30S ribosomal protein S18



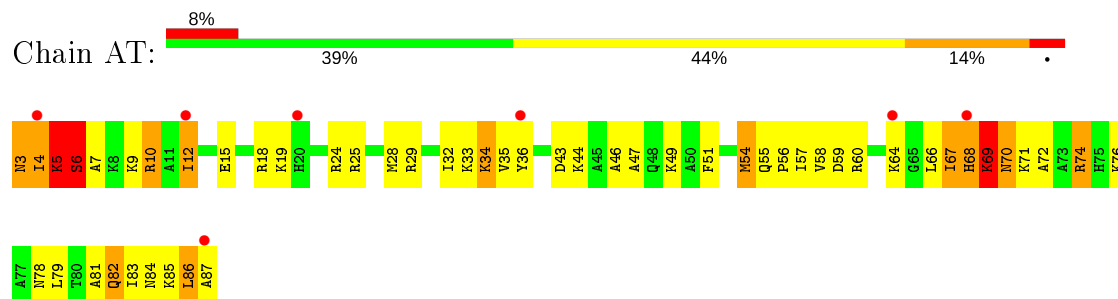
- Molecule 19: 30S ribosomal protein S19



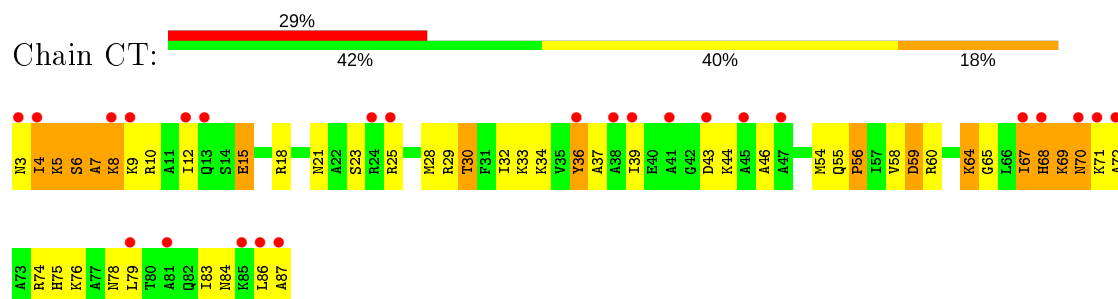
- Molecule 19: 30S ribosomal protein S19



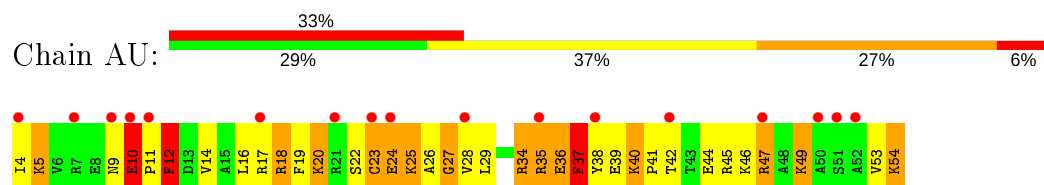
- Molecule 20: 30S ribosomal protein S20



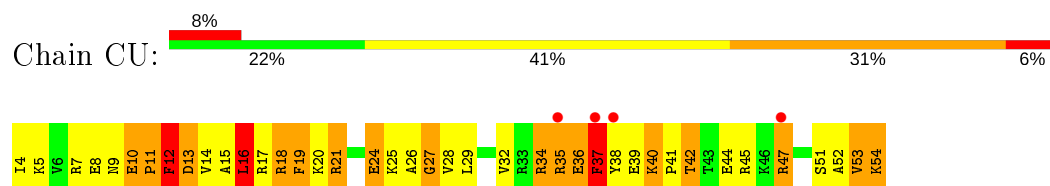
- Molecule 20: 30S ribosomal protein S20



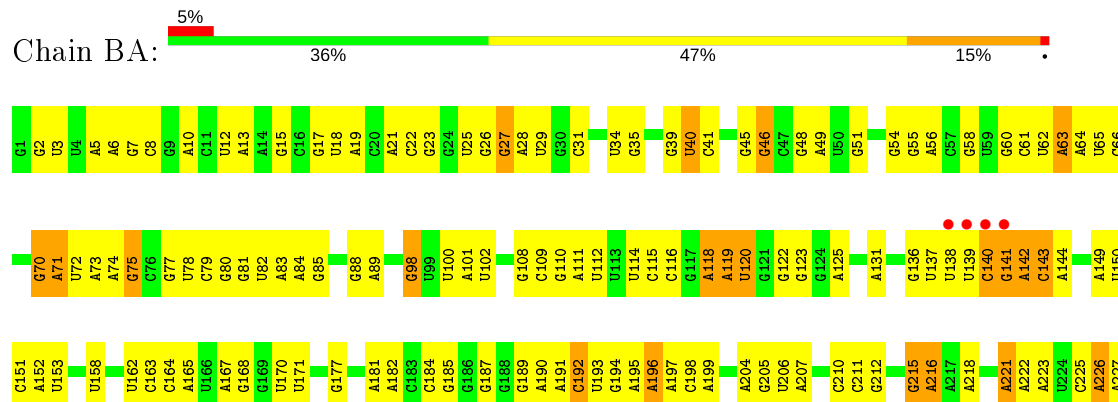
- Molecule 21: 30S ribosomal protein S21



- Molecule 21: 30S ribosomal protein S21

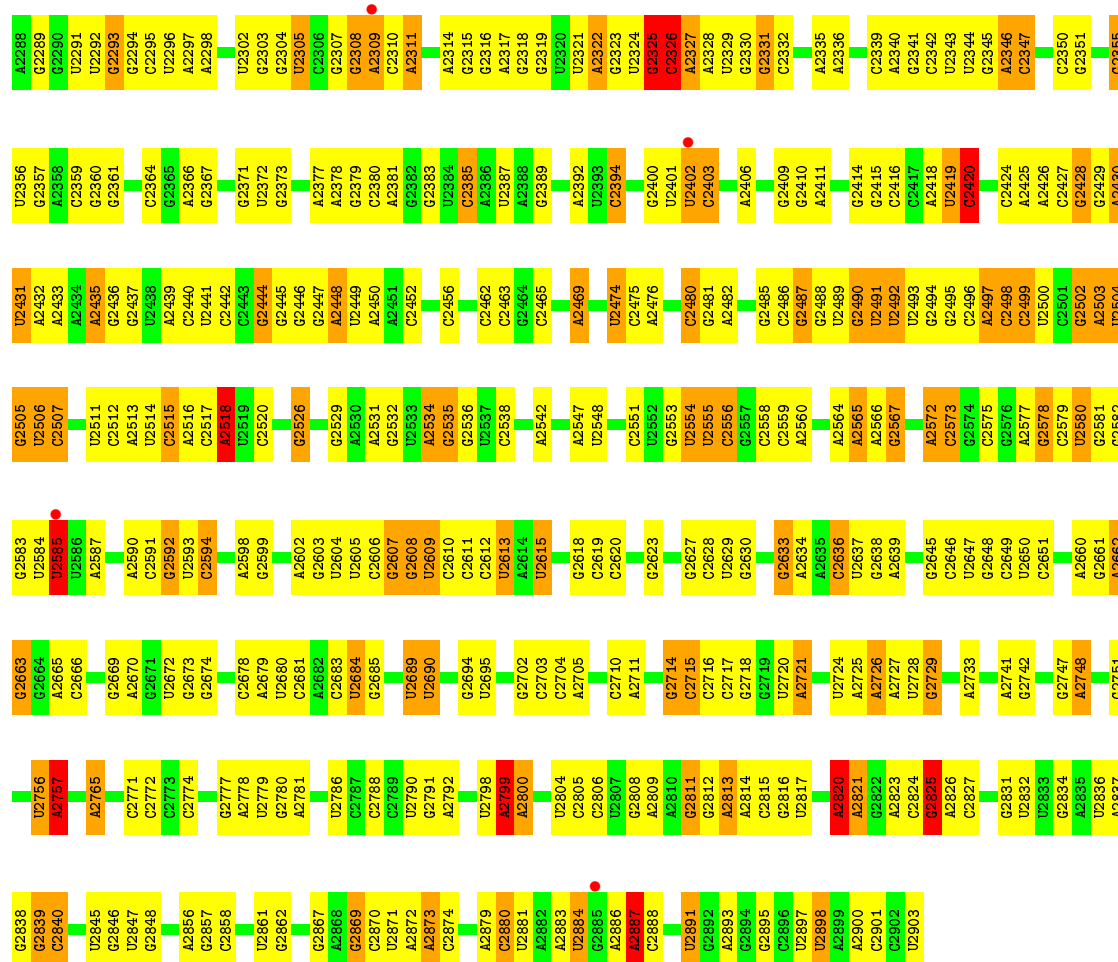


- Molecule 22: 23S rRNA

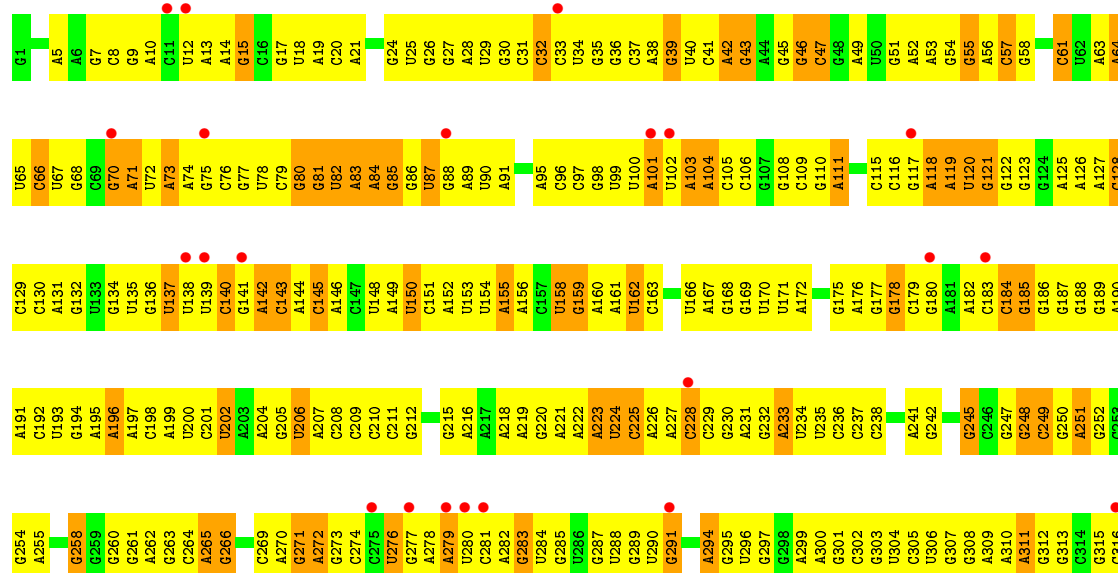


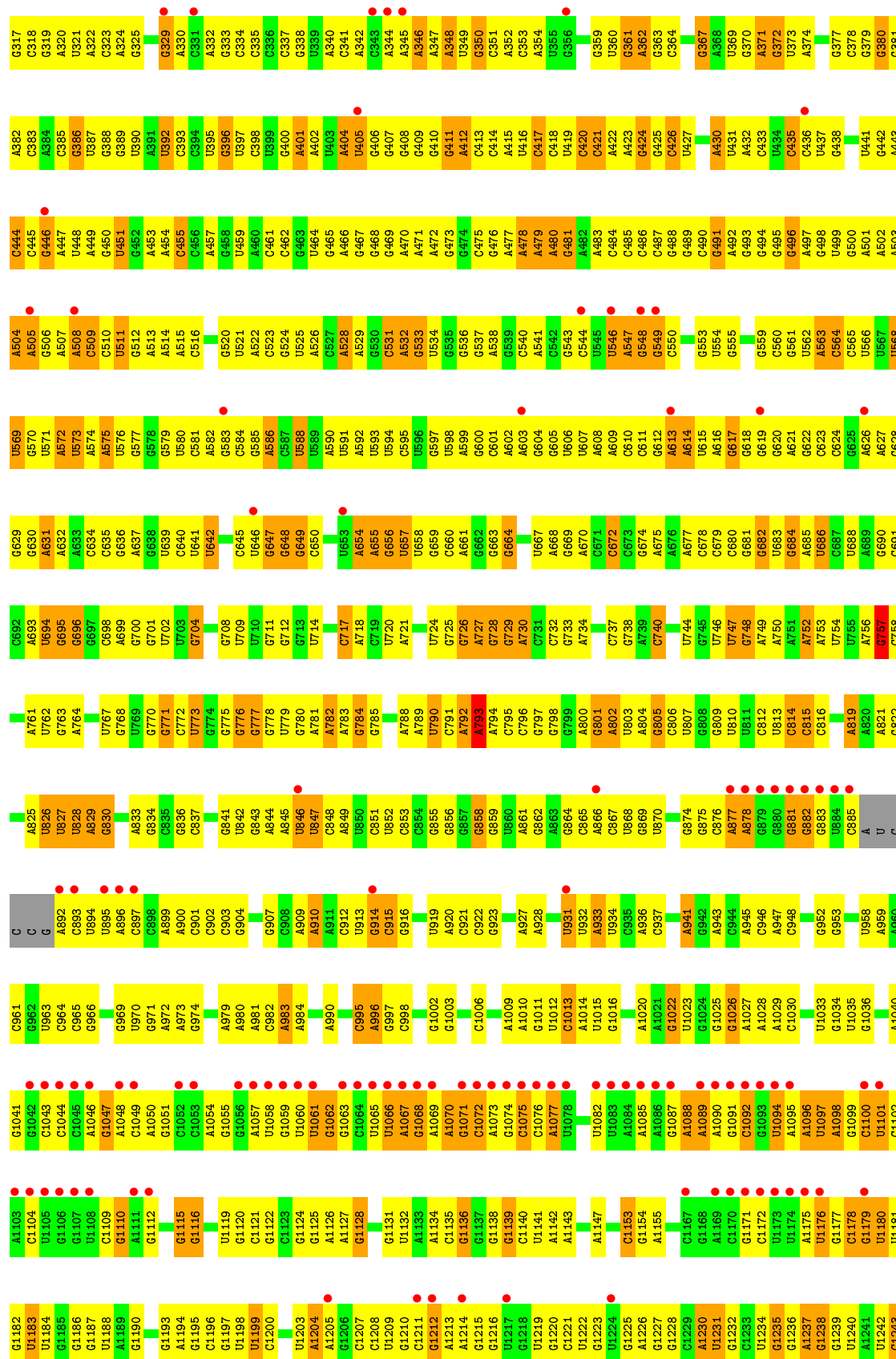


|       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       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| C2214 | C2215 | G2216 | G2217 | G2218 | G2219 | G2220 | G2221 | G2222 | G2223 | G2224 | G2225 | G2226 | G2227 | G2228 | G2229 | G2230 | G2231 | G2232 | G2233 | G2234 | G2235 | G2236 | G2237 | G2238 | G2239 | G2240 | G2241 | G2242 | G2243 | G2244 | G2245 | G2246 | G2247 | G2248 | G2249 | G2250 | G2251 | G2252 | G2253 | G2254 | G2255 | G2256 | G2257 | G2258 | G2259 | G2260 | G2261 | G2262 | G2263 | G2264 | G2265 | G2266 | G2267 | G2268 | G2269 | G2270 | G2271 | G2272 | G2273 | G2274 | G2275 | G2276 | G2277 | G2278 | G2279 | G2280 | G2281 | G2282 | G2283 | G2284 | G2285 | G2286 | G2287 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       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| U1325 | U1326 | U1327 | U1328 | U1329 | U1330 | U1331 | U1332 | U1333 | U1334 | U1335 | U1336 | U1337 | U1338 | U1339 | U1340 | U1341 | U1342 | U1343 | U1344 | U1345 | U1346 | U1347 | U1348 | U1349 | U1350 | U1351 | U1352 | U1353 | U1354 | U1355 | U1356 | U1357 | U1358 | U1359 | U1360 | U1361 | U1362 | U1363 | U1364 | U1365 | U1366 | U1367 | U1368 | U1369 | U1370 | U1371 | U1372 | U1373 | U1374 | U1375 | U1376 | U1377 | U1378 | U1379 | U1380 | U1381 | U1382 | U1383 | U1384 | U1385 | U1386 | U1387 | U1388 | U1389 | U1390 | U1391 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       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| A1392 | A1393 | A1394 | A1395 | A1396 | A1397 |       | G1401 | U1402 | A1403 | A1404 | U1405 | U1406 | U1407 | U1408 | U1409 | G1410 | U1411 | U1412 | A1413 | A1414 | U1415 | U1416 | U1417 | U1418 | U1419 | U1420 | A1421 | U1422 | U1423 | U1424 | U1425 | G1426 | A1427 | U1428 | U1429 | U1430 | U1431 | G1432 | A1433 | U1434 | U1435 | U1436 | U1437 | U1438 | U1439 | U1440 | U1441 | U1442 | U1443 | U1444 | U1445 | 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 | U1482 | U1483 | U1484 | U1485 | U1486 | U1487 | U1488 | U1489 | U1490 | U1491 | U1492 | U1493 | U1494 | U1495 | U1496 | U1497 | U1498 | U1499 | U1500 | U1501 | U1502 | U1503 | U1504 | U1505 | U1506 | U1507 | U1508 | U1509 | U1510 | U1511 | U1512 | U1513 | U1514 | U1515 | U1516 | U1517 | U1518 | U1519 | U1520 | U1521 | U1522 | U1523 | U1524 | U1525 | U1526 | U1527 | U1528 | U1529 | U1530 | U1531 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       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| C1454 | G1455 | G1456 | G1457 | U1458 | U1397 |       | G1464 | G1465 | U1466 | U1467 | U1468 | U1469 | U1470 | G1471 | G1472 | G1473 | U1474 | G1475 |       |       | G1478 | U1554 | U1479 | U1414 | C1458 | U1415 | C1456 | U1481 | G1482 | U1483 | U1484 | U1485 | U1486 | U1487 | C1488 | U1489 | U1490 | U1491 | U1492 | U1493 | U1494 | U1495 | U1496 |       | U1499 | U1500 | U1501 | U1502 | U1503 | U1438 | A1504 |       | U1507 | U1508 | U1509 | U1510 | U1511 | G1512 | U1513 | U1514 | U1515 | U1516 | U1517 | U1518 | U1519 | U1520 | U1521 | U1522 | U1523 | U1524 | U1525 | U1526 | U1527 | U1528 | U1529 | U1530 | U1531 |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       |       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| U2043 | U2044 | U2045 | U2046 | U2047 | U2048 | U2049 | U2050 | U2051 | U2052 | U2053 | U2054 | U2055 | U2056 | U2057 | U2058 | U2059 | U2060 | U2061 | U2062 | U2063 | U2064 | U2065 | U2066 | U2067 | U2068 | U2069 | U2070 | U2071 | U2072 | U2073 | U2074 | U2075 | U2076 | U2077 | U2078 | U2079 | U2080 | U2081 | U2082 | U2083 | U2084 | U2085 | U2086 | U2087 | U2088 | U2089 | U2090 | U2091 | U2092 | U2093 | U2094 | U2095 | U2096 | U2097 | U2098 | U2099 | U2100 | U2101 | U2102 | U2103 | U2104 | U2105 | U2106 | U2107 | U2108 | U2109 | U2110 | U2111 | U2112 | U2113 | U2114 | U2115 | U2116 | U2117 | U2118 | U2119 | U2120 | U2121 | U2122 | U2123 | U2124 | U2125 | U2126 | U2127 | U2128 | U2129 | U2130 | U2131 | U2132 | U2133 | U2134 | U2135 | U2136 | U2137 | U2138 | U2139 | U2140 | U2141 | U2142 | U2143 | U2144 | U2145 | U2146 | U2147 | U2148 | U2149 | U2150 | U2151 | U2152 | U2153 | U2154 | U2155 | U2156 | U2157 | U2158 | U2159 | U2160 | U2161 | U2162 | U2163 | U2164 | U2165 | U2166 | U2167 | U2168 | U2169 | U2170 | U2171 | U2172 | U2173 | U2174 | U2175 | U2176 | U2177 | U2178 | U2179 | U2180 | U2181 | U2182 | U2183 | U2184 | U2185 | U2186 | U2187 | U2188 | U2189 | U2190 | U2191 | U2192 | U2193 | U2194 | U2195 | U2196 | U2197 | U2198 | U2199 | U2200 | U2201 | U2202 | U2203 | U2204 | U2205 | U2206 | U2207 | U2208 | U2209 | U2210 | U2211 | U2212 | U2213 | U2214 | U2215 | U2216 | U2217 | U2218 | U2219 | U2220 | U2221 | U2222 | U2223 | U2224 | U2225 | U2226 | U2227 | U2228 | U2229 | U2230 | U2231 | U2232 | U2233 | U2234 | U2235 | U2236 | U2237 | U2238 | U2239 | U2240 | U2241 | U2242 | U2243 | U2244 | U2245 | U2246 | U2247 | U2248 | U2249 | U2250 | U2251 | U2252 | U2253 | U2254 | U2255 | U2256 | U2257 | U2258 | U2259 | U2260 | U2261 | U2262 | U2263 | U2264 | U2265 | U2266 | U2267 | U2268 | U2269 | U2270 | U2271 | U2272 | U2273 | U2274 | U2275 | U2276 | U2277 | U2278 | U2279 | U2280 | U2281 | U2282 | U2283 | U2284 | U2285 | U2286 | U2287 |



• Molecule 22: 23S rRNA



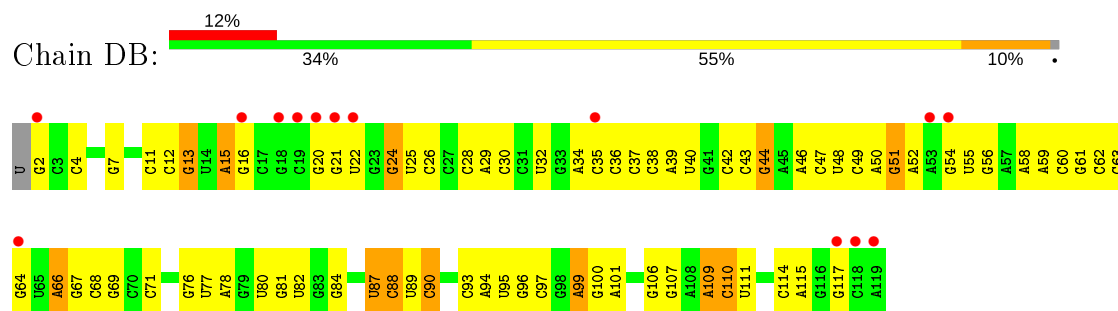


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| G2124 | G2056 | G1992 | A1853 | C1790 | G1724 | G1649 | C1575 | G1510 | A1439 | G1371 | G1311 | A1244 |
| G2125 | G2057 | U1993 | A1854 | A1791 | U1725 | A1650 | U1576 | G1511 | U1440 | U1372 | U1312 | G1245 |
| G2126 | A2058 | G1994 | U1855 | G1792 | C1726 | G1651 | G1578 | U1512 | G1441 | G1373 | U1313 | A1246 |
| G2127 | A2059 | U1995 | U1856 | C1793 | C1727 | A1652 | U1578 | U1513 | U1442 | A1374 | G1314 | A1247 |
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| G2129 | G2061 | C1997 | A1858 | U1729 | C1729 | A1654 | G1581 | A1515 | G1444 | C1376 | U1316 | U1249 |
| U2130 | A2062 | A1998 | U1859 | G1797 | C1730 | A1655 | C1582 | G1519 | G1445 | G1377 | U1317 | G1250 |
| U2131 | C2063 | G1999 | G1860 | U1798 | G1731 | A1656 | A1583 | G1520 | G1446 | A1378 | U1318 | C1251 |
| U2132 | C2064 | C2001 | G1861 | U1799 | G1732 | U1657 | A1584 | U1520 | C1447 | U1379 | G1319 | G1252 |
| C2065 | C2065 | C2001 | G1862 | G1800 | G1733 | C1658 | C1585 | U1523 | G1448 | G1380 | C1320 | A1253 |
| C2066 | C2066 | C2001 | G1863 | A1801 | G1734 | G1659 | A1586 | U1524 | G1381 | G1381 | A1321 | A1254 |
| G2067 | G2067 | A2004 | U1864 | A1802 | A1735 | G1660 | G1587 | G1525 | G1382 | G1382 | A1322 | U1255 |
| U2068 | G2068 | C2006 | U1865 | A1803 | U1736 | G1661 | G1588 | A1526 | G1383 | G1383 | G1323 | U1256 |
| G2069 | G2069 | C2006 | A1866 | C1804 | G1737 | U1662 | U1589 | C1526 | G1452 | A1384 | G1324 | C1257 |
| A2070 | A2070 | U2007 | G1867 | A1805 | G1738 | G1663 | A1590 | G1527 | C1454 | U1390 | U1325 | U1258 |
| A2071 | A2071 | C2008 | G1868 | C1806 | A1739 | A1664 | A1591 | U1528 | G1455 | U1326 | U1326 | G1259 |
| C2072 | C2072 | G2010 | G1869 | G1807 | G1740 | A1665 | C1592 | G1529 | G1456 | A1327 | A1327 | A1260 |
| C2073 | C2073 | G2010 | G1870 | A1808 | C1741 | G1666 | A1593 | G1530 | U1457 | A1392 | A1328 | C1261 |
| U2074 | U2074 | U2011 | A1871 | A1809 | U1742 | G1667 | U1594 | C1531 | U1458 | A1393 | U1329 | A1262 |
| U2075 | U2075 | G2012 | A1872 | A1810 | G1743 | A1668 | C1595 | A1532 | U1459 | U1394 | C1330 | U1263 |
| C2145 | C2145 | A2013 | G1873 | G1811 | A1744 | A1669 | A1596 | C1533 | U1460 | A1395 | G1331 | A1264 |
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| C2150 | C2150 | G2018 | G1878 | C1816 | C1752 | G1674 | G1601 | G1538 | G1465 | U1400 | A1336 | A1269 |
| U2151 | U2151 | A2019 | C1879 | G1817 | C1753 | C1675 | U1602 | U1539 | U1466 | G1401 | G1337 | G1270 |
| G2152 | G2152 | A2020 | A1880 | U1818 | A1754 | A1676 | U1603 | G1540 | U1467 | U1402 | G1338 | G1271 |
| G2156 | G2156 | C2021 | C1881 | A1819 | A1755 | A1677 | C1604 | C1541 | U1468 | A1403 | G1339 | A1272 |
| G2157 | G2157 | U2022 | U1882 | U1820 | G1756 | A1678 | G1605 | U1542 | A1469 | C1404 | U1340 | U1273 |
| A2158 | A2158 | C2023 | G1883 | A1821 | A1757 | A1679 | C1606 | G1543 | A1470 | U1405 | G1341 | A1274 |
| G2159 | G2159 | G2024 | G1884 | C1822 | U1758 | U1680 | C1607 | A1544 | G1471 | U1406 | A1342 | A1275 |
| C2160 | C2160 | C2025 | A1885 | G1823 | A1759 | G1681 | A1608 | U1545 | G1472 | G1407 | G1343 | A1276 |
| C2161 | C2161 | U2026 | A1886 | G1824 | C1760 | G1682 | A1609 | G1546 | U1476 | U1409 | G1344 | G1277 |
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| A2163 | A2163 | A2030 | G1890 | G1826 | U1764 | U1688 | G1613 | U1551 | C1480 | U1411 | G1346 | G1280 |
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| U2167 | U2167 | A2033 | G1896 | A1829 | G1767 | U1693 | A1618 | U1554 | G1483 | G1416 | C1350 | A1286 |
| G2168 | G2168 | U2034 | G1897 | G1831 | G1768 | C1694 | U1555 | G1556 | U1484 | C1417 | C1351 | A1287 |
| A2169 | A2169 | G2035 | U1898 | G1832 | U1769 | G1695 | G1556 | C1557 | U1485 | G1418 | U1352 | G1288 |
| C2170 | C2170 | A1970 | A1899 | C1833 | U1773 | U1698 | U1621 | C1557 | U1486 | A1419 | A1353 | C1289 |
| U2106 | U2106 | G1972 | G1903 | U1834 | C1774 | A1698 | G1622 | C1557 | U1487 | A1420 | A1354 | C1293 |
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| A2108 | A2108 | G1975 | G1905 | C1836 | G1776 | U1708 | C1625 | U1559 | C1489 | G1426 | C1357 | G1297 |
| G2110 | G2110 | U2041 | G1906 | C1837 | U1777 | U1709 | A1626 | C1561 | G1489 | G1427 | C1358 | C1298 |
| U2111 | U2111 | A1978 | G1907 | G1838 | U1778 | G1710 | G1627 | U1562 | U1490 | A1428 | A1359 | C1299 |
| C2175 | C2175 | U1979 | G1907 | G1839 | U1779 | A1711 | G1628 | U1563 | G1493 | C1428 | G1360 | G1300 |
| U2113 | U2113 | G1980 | U1911 | C1843 | U1780 | U1712 | C1638 | C1564 | G1500 | G1429 | G1361 | G1301 |
| C2044 | C2044 | A1981 | A1912 | C1844 | A1781 | A1713 | C1639 | C1565 | G1501 | G1430 | C1362 | A1304 |
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| G2208 | G2208 | G1983 | C1914 | G1846 | A1783 | G1715 | A1641 | G1568 | A1503 | G1432 | G1364 | C1306 |
| C2209 | C2209 | A1915 | U1915 | A1847 | A1784 | U1716 | A1641 | G1569 | A1504 | A1433 | A1365 | A1307 |
| U2118 | U2118 | C1985 | A1916 | A1848 | A1785 | A1717 | G1645 | A1570 | U1506 | G1435 | A1366 | A1308 |
| A2119 | A2119 | C1986 | U1917 | G1849 | A1786 | G1718 | C1646 | A1571 | U1507 | G1436 | G1367 | G1309 |
| G2210 | G2210 | G1989 | A1918 | C1850 | A1787 | U1722 | U1647 | U1571 | A1508 | A1437 | G1368 | A1310 |
| C2211 | C2211 | C1990 | A1919 | U1851 | A1788 | A1722 | U1648 | C1574 | A1509 | U1438 | C1370 |       |
| U2122 | U2122 | C2054 | C1920 | U1852 | A1789 | G1723 |       |       |       |       |       |       |
| G2182 | G2182 | C2055 |       |       |       |       |       |       |       |       |       |       |
| G2183 | G2183 | C2056 |       |       |       |       |       |       |       |       |       |       |
| A2184 | A2184 | C2057 |       |       |       |       |       |       |       |       |       |       |
| U2185 | U2185 | C2058 |       |       |       |       |       |       |       |       |       |       |
| G2186 | G2186 | C2059 |       |       |       |       |       |       |       |       |       |       |
| G2187 | G2187 | C2060 |       |       |       |       |       |       |       |       |       |       |
| G2188 | G2188 | C2061 |       |       |       |       |       |       |       |       |       |       |
| G2189 | G2189 | C2062 |       |       |       |       |       |       |       |       |       |       |
| G2190 | G2190 | C2063 |       |       |       |       |       |       |       |       |       |       |
| G2191 | G2191 | C2064 |       |       |       |       |       |       |       |       |       |       |
| G2192 | G2192 | C2065 |       |       |       |       |       |       |       |       |       |       |
| G2193 | G2193 | C2066 |       |       |       |       |       |       |       |       |       |       |
| G2194 | G2194 | C2067 |       |       |       |       |       |       |       |       |       |       |
| G2195 | G2195 | C2068 |       |       |       |       |       |       |       |       |       |       |
| G2196 | G2196 | C2069 |       |       |       |       |       |       |       |       |       |       |
| G2197 | G2197 | C2070 |       |       |       |       |       |       |       |       |       |       |
| G2198 | G2198 | C2071 |       |       |       |       |       |       |       |       |       |       |
| G2199 | G2199 | C2072 |       |       |       |       |       |       |       |       |       |       |
| G2200 | G2200 | C2073 |       |       |       |       |       |       |       |       |       |       |
| G2201 | G2201 | C2074 |       |       |       |       |       |       |       |       |       |       |
| G2202 | G2202 | C2075 |       |       |       |       |       |       |       |       |       |       |
| G2203 | G2203 | C2076 |       |       |       |       |       |       |       |       |       |       |
| G2204 | G2204 | C2077 |       |       |       |       |       |       |       |       |       |       |
| G2205 | G2205 | C2078 |       |       |       |       |       |       |       |       |       |       |
| G2206 | G2206 | C2079 |       |       |       |       |       |       |       |       |       |       |
| G2207 | G2207 | C2080 |       |       |       |       |       |       |       |       |       |       |
| G2208 | G2208 | C2081 |       |       |       |       |       |       |       |       |       |       |
| G2209 | G2209 | C2082 |       |       |       |       |       |       |       |       |       |       |
| G2210 | G2210 | C2083 |       |       |       |       |       |       |       |       |       |       |
| G2211 | G2211 | C2084 |       |       |       |       |       |       |       |       |       |       |
| G2212 | G2212 | C2085 |       |       |       |       |       |       |       |       |       |       |
| G2213 | G2213 | C2086 |       |       |       |       |       |       |       |       |       |       |
| G2214 | G2214 | C2087 |       |       |       |       |       |       |       |       |       |       |
| G2215 | G2215 | C2088 |       |       |       |       |       |       |       |       |       |       |
| G2216 | G2216 | C2089 |       |       |       |       |       |       |       |       |       |       |
| G2217 | G2217 | C2090 |       |       |       |       |       |       |       |       |       |       |
| G2218 | G2218 | C2091 |       |       |       |       |       |       |       |       |       |       |
| G2219 | G2219 | C2092 |       |       |       |       |       |       |       |       |       |       |
| G2220 | G2220 | C2093 |       |       |       |       |       |       |       |       |       |       |
| G2221 | G2221 | C2094 |       |       |       |       |       |       |       |       |       |       |
| G2222 | G2222 | C2095 |       |       |       |       |       |       |       |       |       |       |
| G2223 | G2223 | C2096 |       |       |       |       |       |       |       |       |       |       |
| G2224 | G2224 | C2097 |       |       |       |       |       |       |       |       |       |       |
| G2225 | G2225 | C2098 |       |       |       |       |       |       |       |       |       |       |
| G2226 | G2226 | C2099 |       |       |       |       |       |       |       |       |       |       |
| G2227 | G2227 | C2100 |       |       |       |       |       |       |       |       |       |       |
| G2228 | G2228 | C2101 |       |       |       |       |       |       |       |       |       |       |
| G2229 | G2229 | C2102 |       |       |       |       |       |       |       |       |       |       |
| G2230 | G2230 | C2103 |       |       |       |       |       |       |       |       |       |       |
| G2231 | G2231 | C2104 |       |       |       |       |       |       |       |       |       |       |
| G2232 | G2232 | C2105 |       |       |       |       |       |       |       |       |       |       |
| G2233 | G2233 | C2106 |       |       |       |       |       |       |       |       |       |       |
| G2234 | G2234 | C2107 |       |       |       |       |       |       |       |       |       |       |
| G2235 | G2235 | C2108 |       |       |       |       |       |       |       |       |       |       |
| G2236 | G2236 | C2109 |       |       |       |       |       |       |       |       |       |       |
| G2237 | G2237 | C2110 |       |       |       |       |       |       |       |       |       |       |
| G2238 | G2238 | C2111 |       |       |       |       |       |       |       |       |       |       |
| G2239 | G2239 | C2112 |       |       |       |       |       |       |       |       |       |       |
| G2240 | G2240 | C2113 |       |       |       |       |       |       |       |       |       |       |
| G2241 | G2241 | C2114 |       |       |       |       |       |       |       |       |       |       |
| G2242 | G2242 | C2115 |       |       |       |       |       |       |       |       |       |       |
| G2243 | G2243 | C2116 |       |       |       |       |       |       |       |       |       |       |
| G2244 | G2244 | C2117 |       |       |       |       |       |       |       |       |       |       |
| G2245 | G2245 | C2118 |       |       |       |       |       |       |       |       |       |       |
| G2246 | G2246 | C2119 |       |       |       |       |       |       |       |       |       |       |
| G2247 | G2247 | C2120 |       |       |       |       |       |       |       |       |       |       |
| G2248 | G2248 | C2121 |       |       |       |       |       |       |       |       |       |       |
| G2249 | G2249 | C2122 |       |       |       |       |       |       |       |       |       |       |
| G2250 | G2250 | C2123 |       |       |       |       |       |       |       |       |       |       |

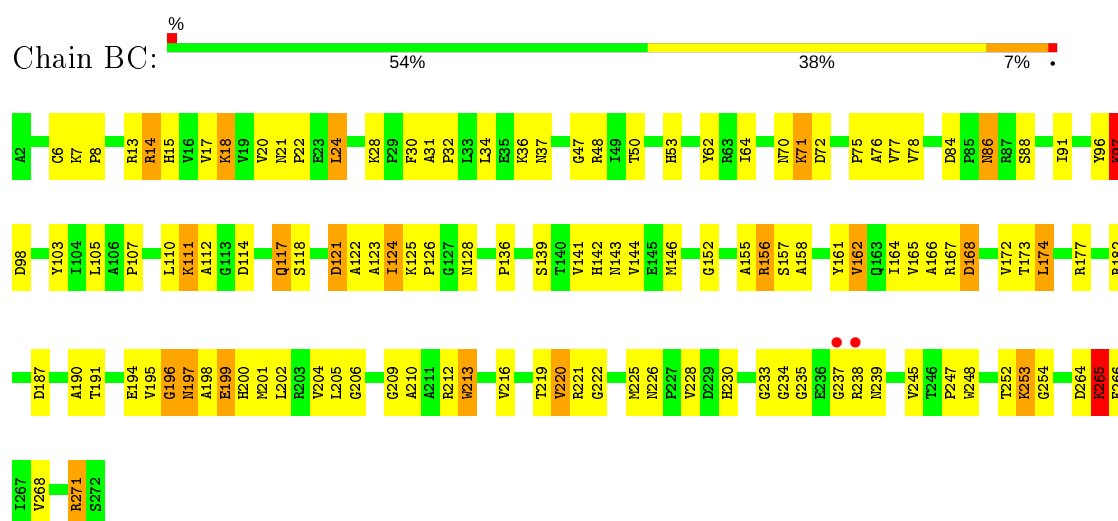




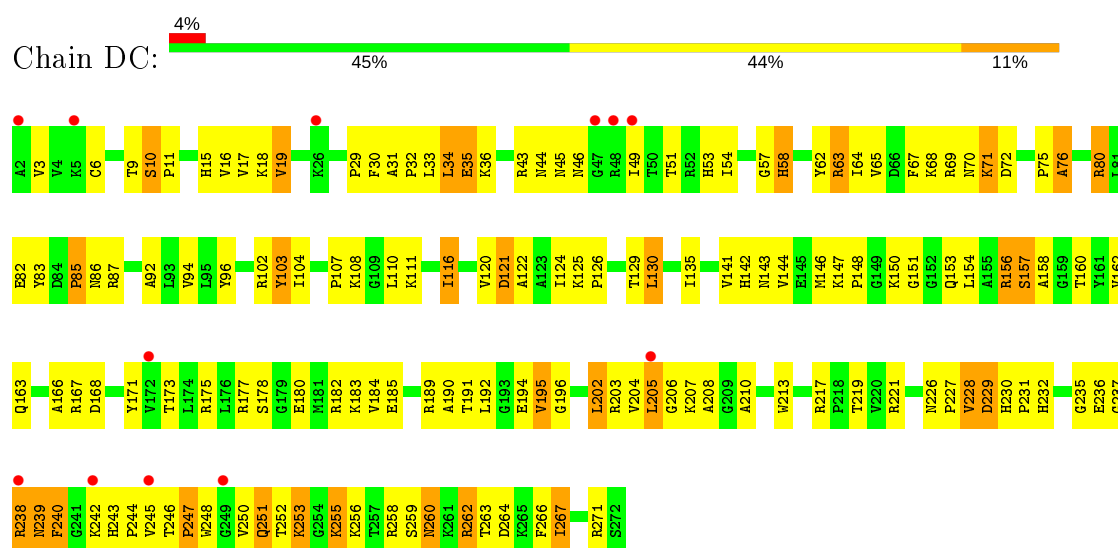
- Molecule 23: 5S rRNA



- Molecule 24: 50S ribosomal protein L2

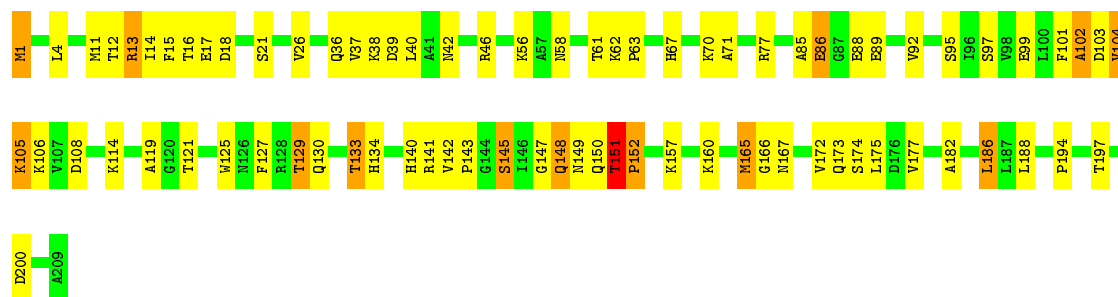


- Molecule 24: 50S ribosomal protein L2

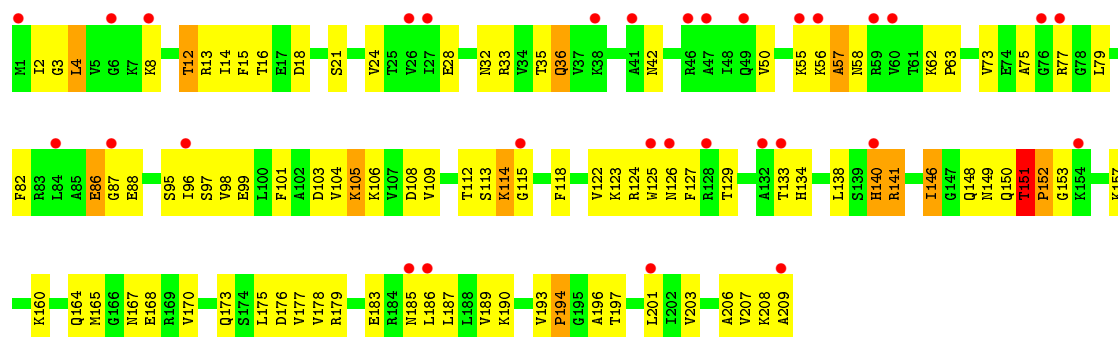


- Molecule 25: 50S ribosomal protein L3

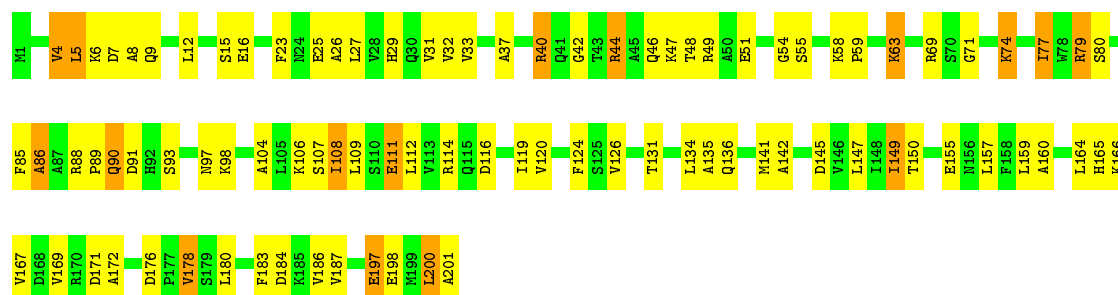




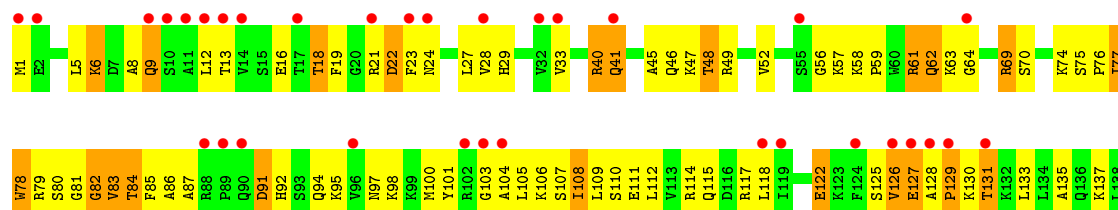
- Molecule 25: 50S ribosomal protein L3

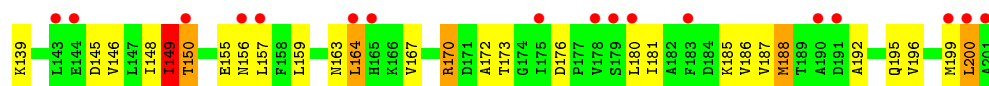


- Molecule 26: 50S ribosomal protein L4

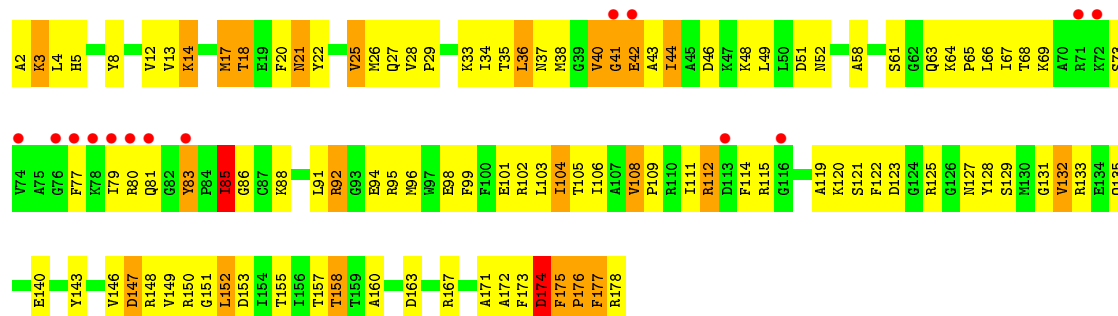


- Molecule 26: 50S ribosomal protein L4

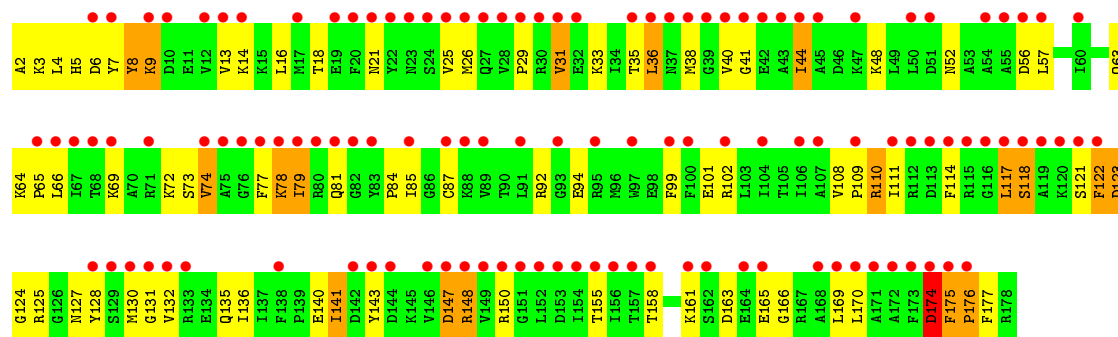




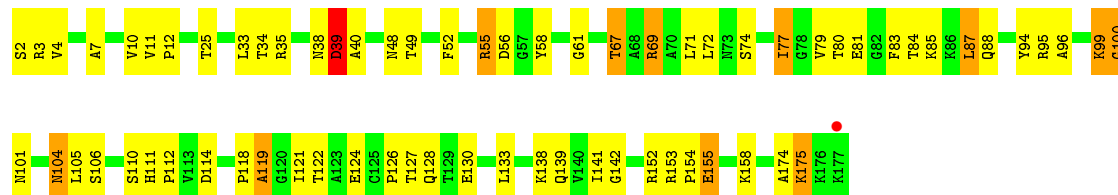
• Molecule 27: 50S ribosomal protein L5



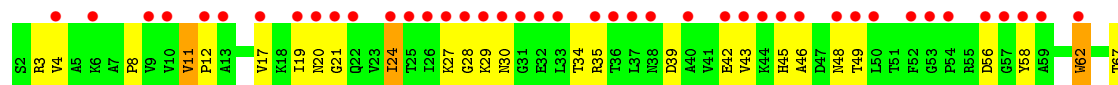
• Molecule 27: 50S ribosomal protein L5

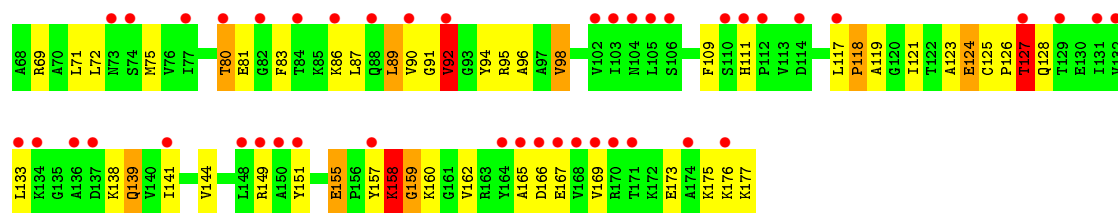


• Molecule 28: 50S ribosomal protein L6

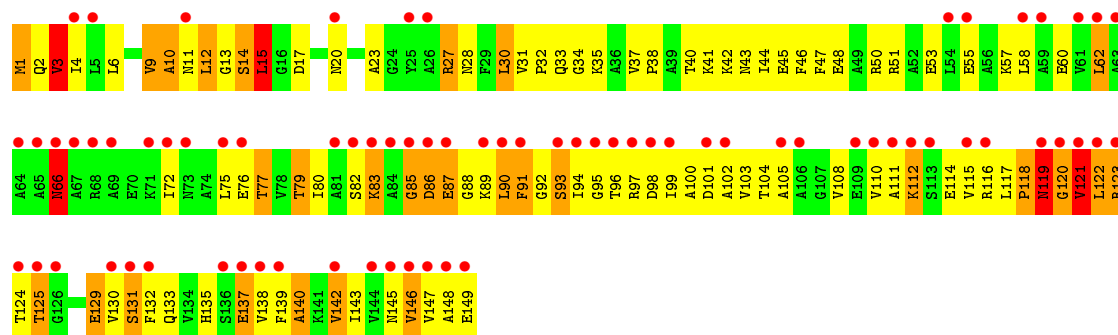


• Molecule 28: 50S ribosomal protein L6

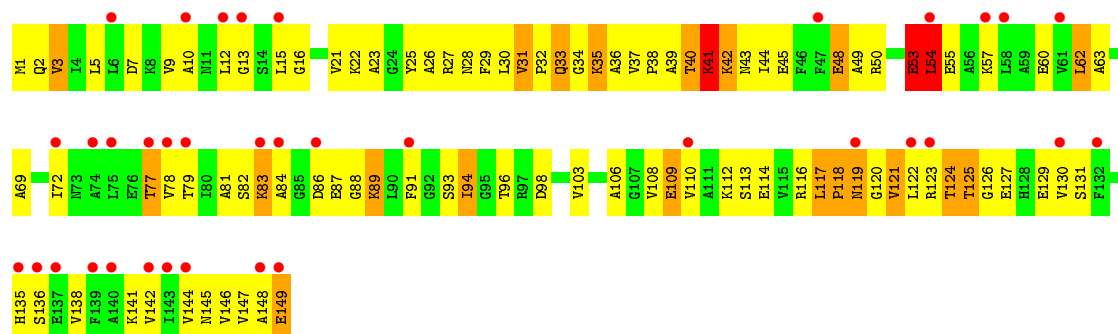




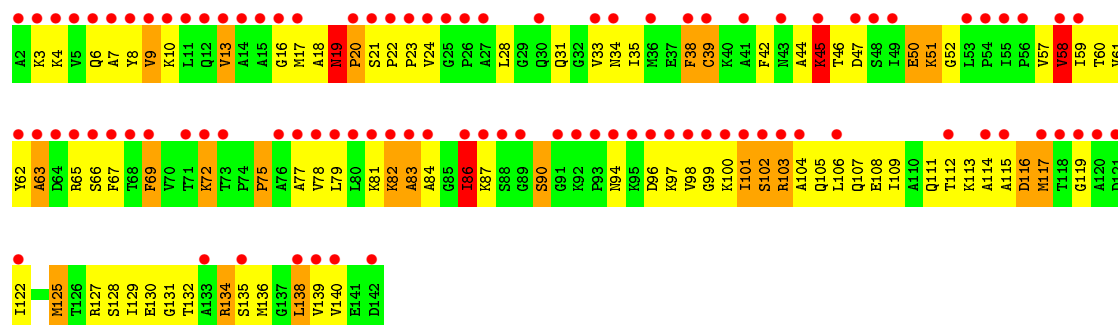
• Molecule 29: 50S ribosomal protein L9



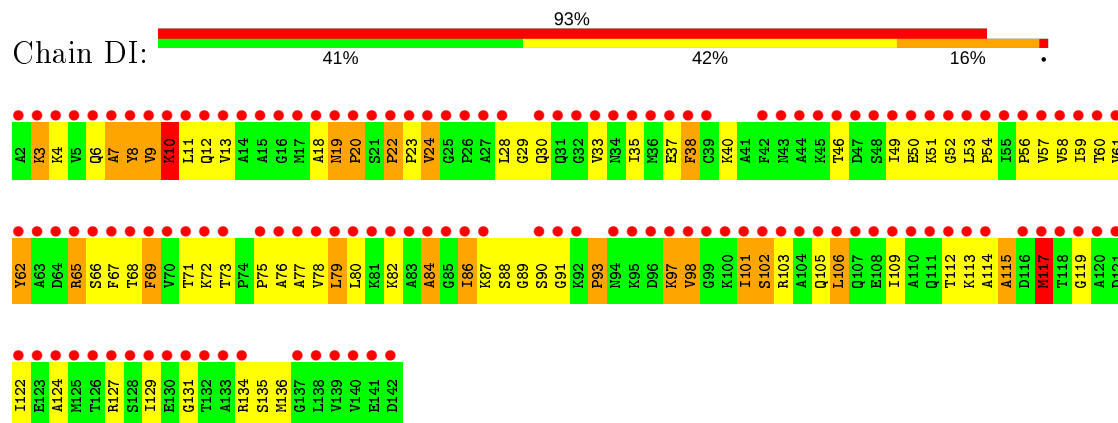
• Molecule 29: 50S ribosomal protein L9



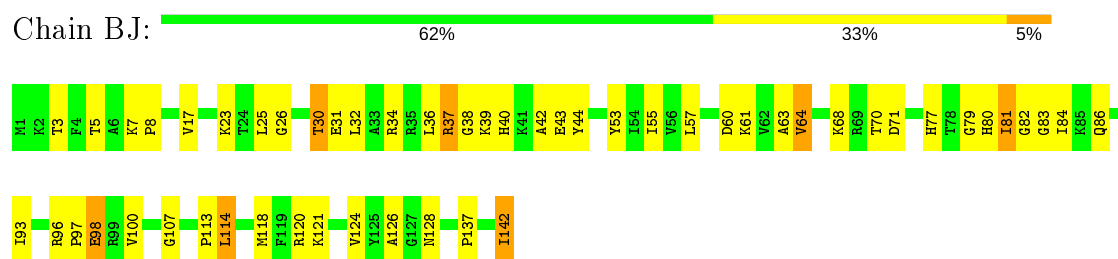
• Molecule 30: 50S ribosomal protein L11



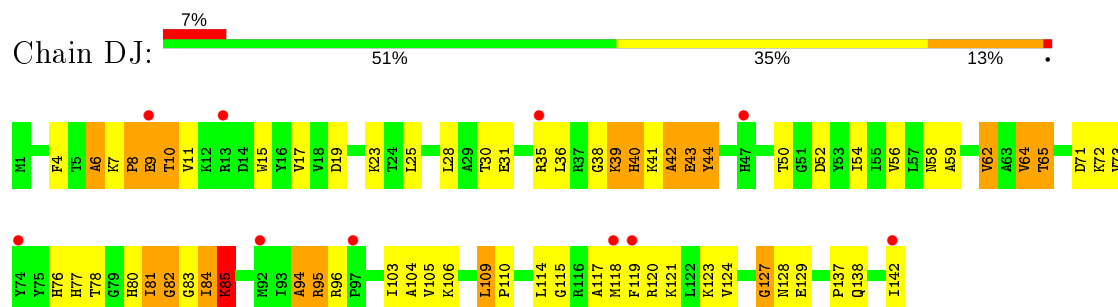
- Molecule 30: 50S ribosomal protein L11



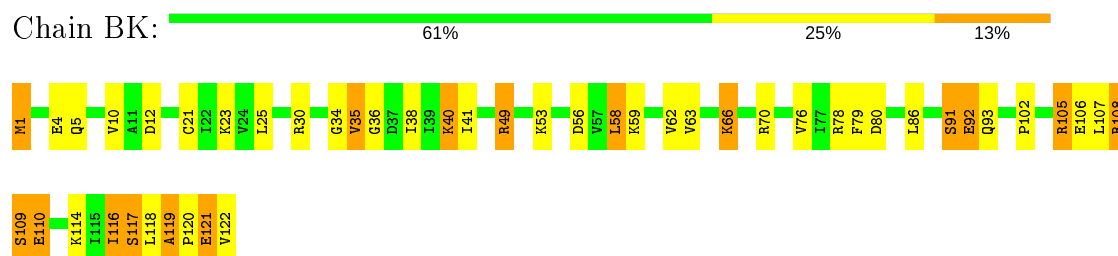
- Molecule 31: 50S ribosomal protein L13



- Molecule 31: 50S ribosomal protein L13

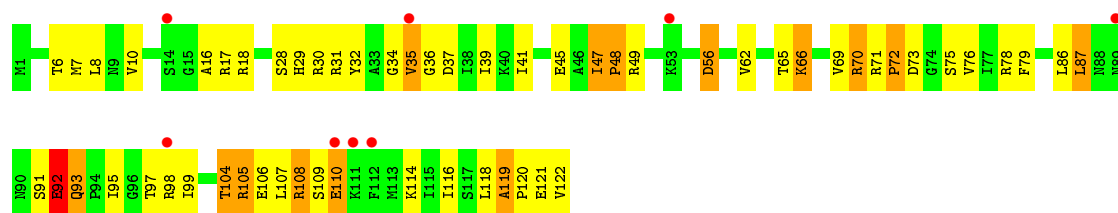


- Molecule 32: 50S ribosomal protein L14



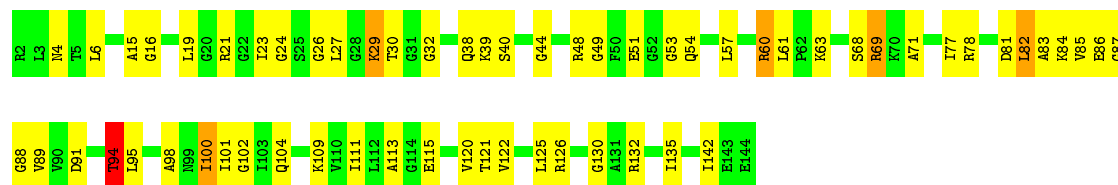
- Molecule 32: 50S ribosomal protein L14





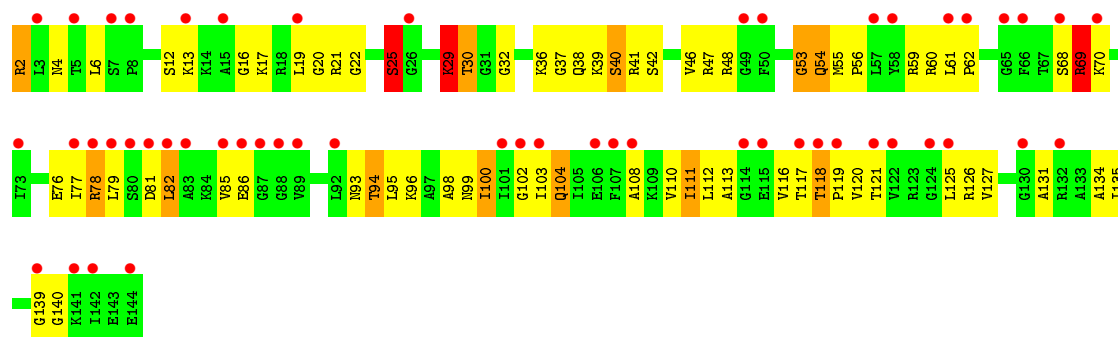
• Molecule 33: 50S ribosomal protein L15

Chain BL: 57% 38% . .



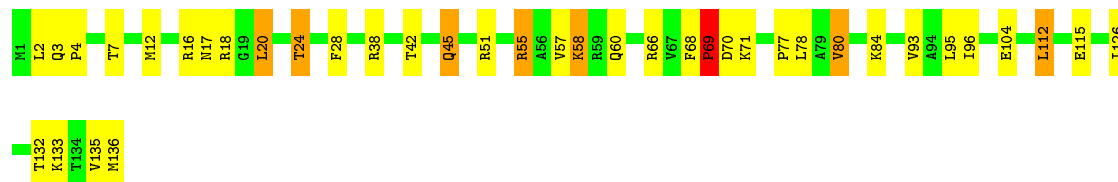
• Molecule 33: 50S ribosomal protein L15

Chain DL: 37% 49% 41% 8% .



• Molecule 34: 50S ribosomal protein L16

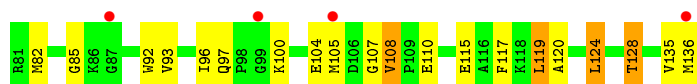
Chain BM: 71% 23% 5% .



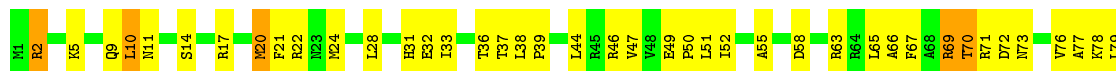
• Molecule 34: 50S ribosomal protein L16

Chain DM: 11% 58% 33% 9%





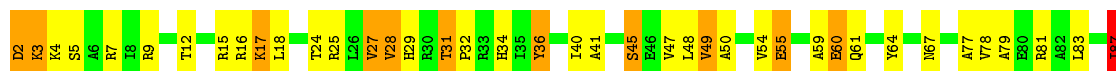
- Molecule 35: 50S ribosomal protein L17



- Molecule 35: 50S ribosomal protein L17



- Molecule 36: 50S ribosomal protein L18

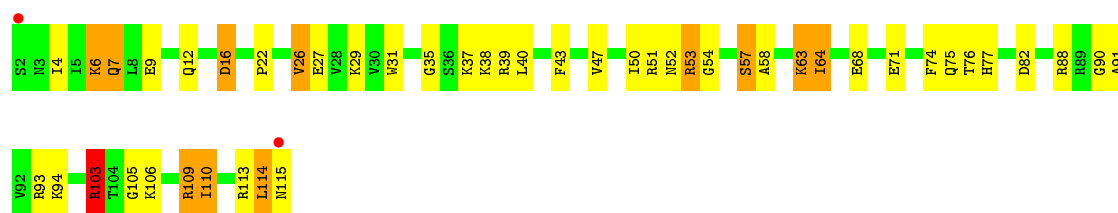


- Molecule 36: 50S ribosomal protein L18

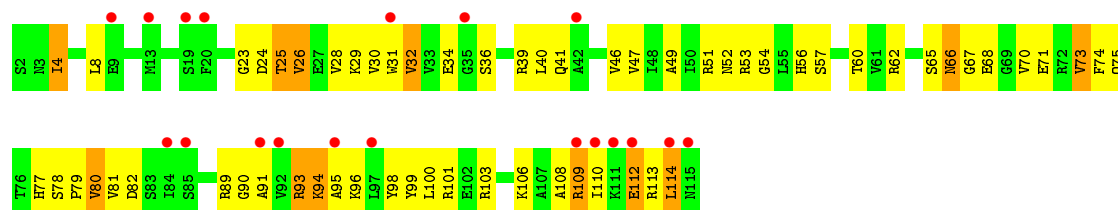


- Molecule 37: 50S ribosomal protein L19

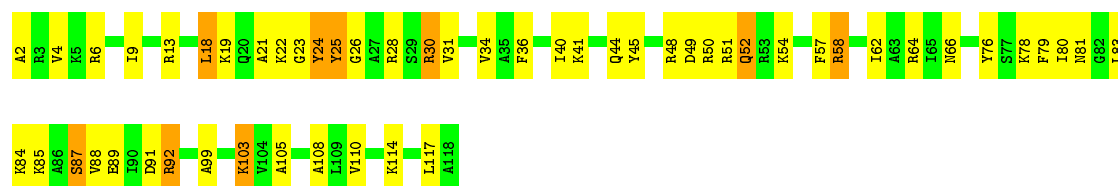




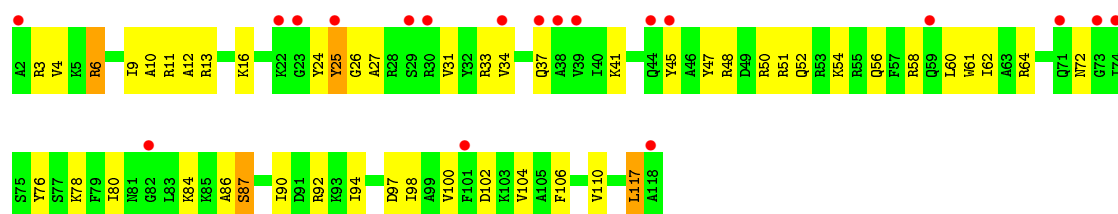
• Molecule 37: 50S ribosomal protein L19



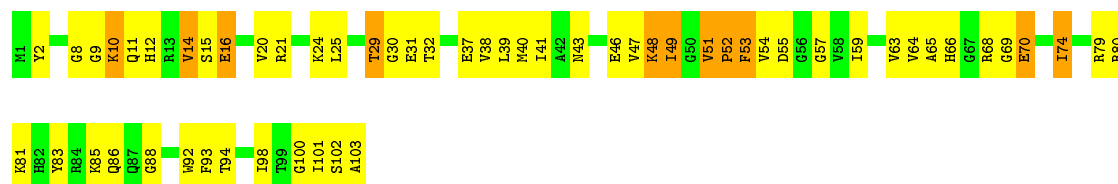
• Molecule 38: 50S ribosomal protein L20



• Molecule 38: 50S ribosomal protein L20

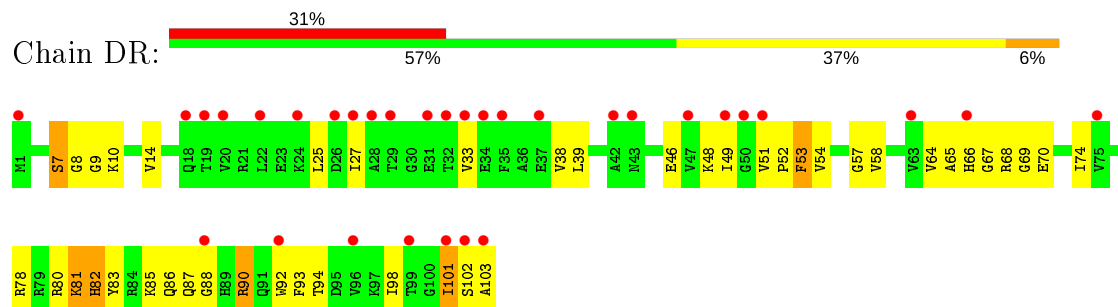


• Molecule 39: 50S ribosomal protein L21

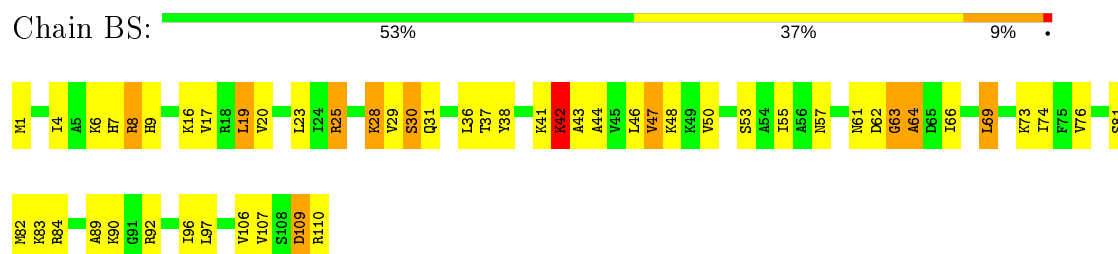




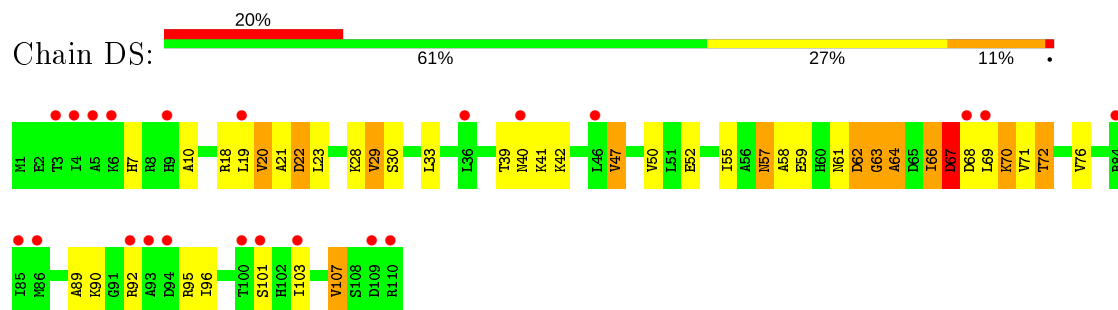
- Molecule 39: 50S ribosomal protein L21



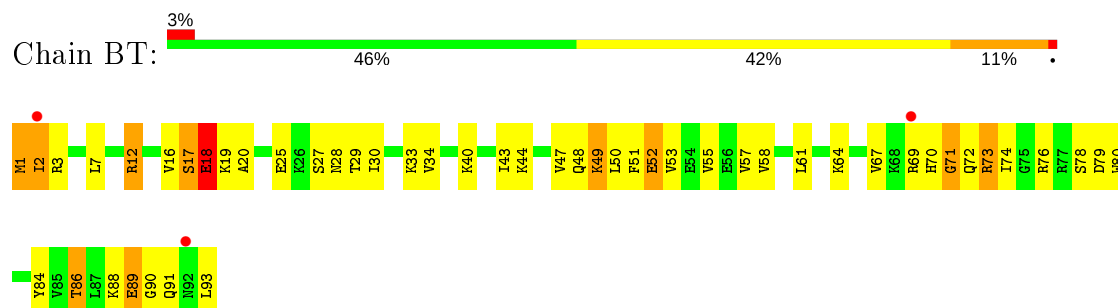
- Molecule 40: 50S ribosomal protein L22



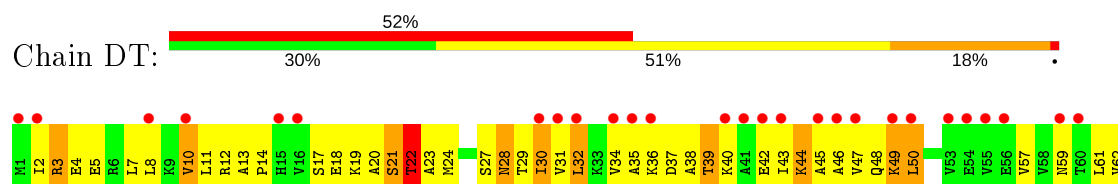
- Molecule 40: 50S ribosomal protein L22

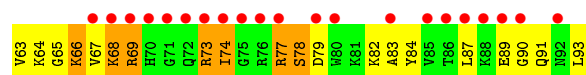


- Molecule 41: 50S ribosomal protein L23

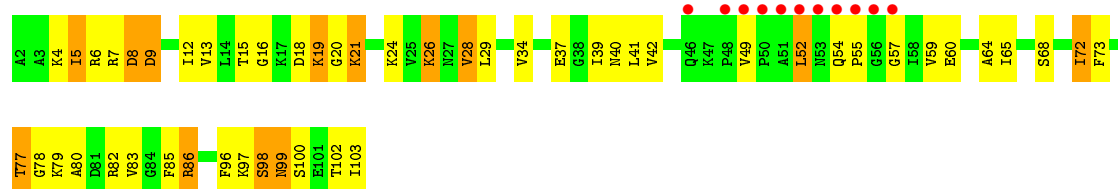


- Molecule 41: 50S ribosomal protein L23

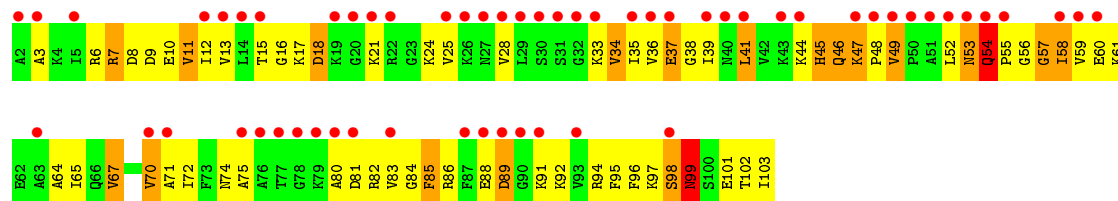




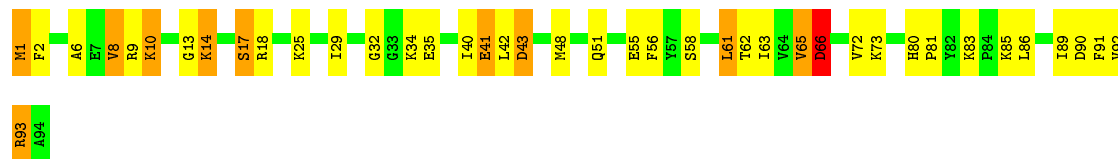
- Molecule 42: 50S ribosomal protein L24



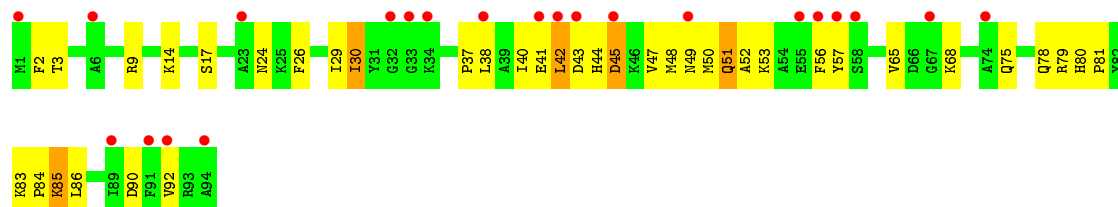
- Molecule 42: 50S ribosomal protein L24



- Molecule 43: 50S ribosomal protein L25

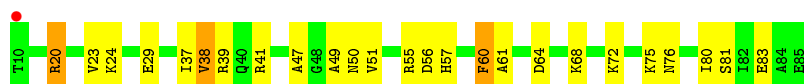


- Molecule 43: 50S ribosomal protein L25

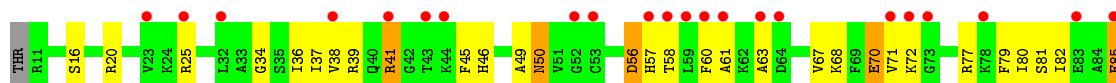


- Molecule 44: 50S ribosomal protein L27





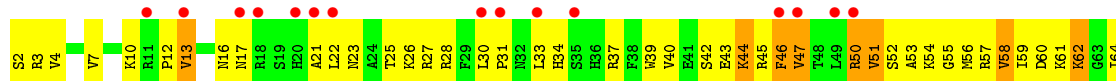
- Molecule 44: 50S ribosomal protein L27



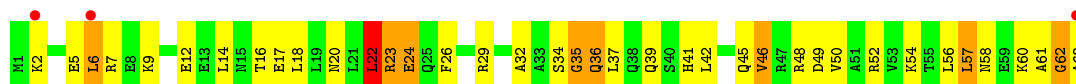
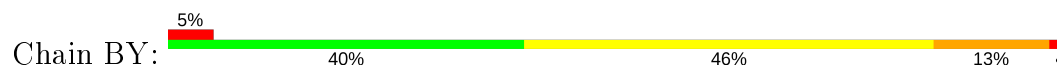
- Molecule 45: 50S ribosomal protein L28



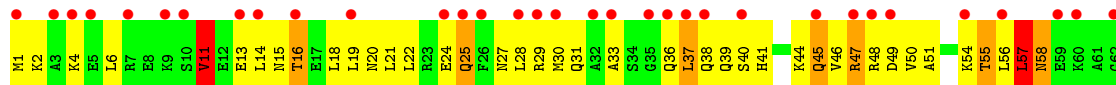
- Molecule 45: 50S ribosomal protein L28



- Molecule 46: 50S ribosomal protein L29



- Molecule 46: 50S ribosomal protein L29



- Molecule 47: 50S ribosomal protein L30

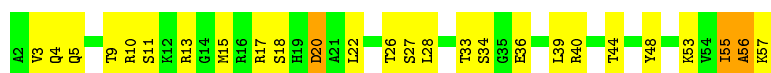




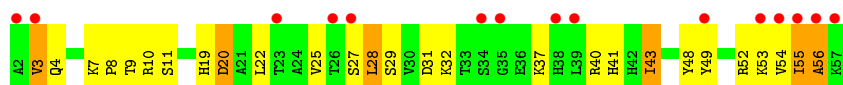
- Molecule 47: 50S ribosomal protein L30



- Molecule 48: 50S ribosomal protein L32



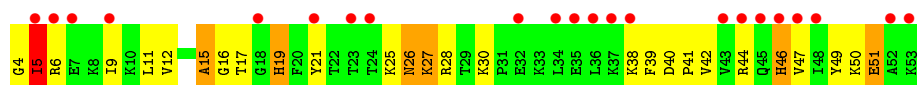
- Molecule 48: 50S ribosomal protein L32



- Molecule 49: 50S ribosomal protein L33



- Molecule 49: 50S ribosomal protein L33

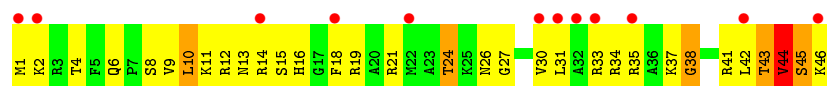


- Molecule 50: 50S ribosomal protein L34



- Molecule 50: 50S ribosomal protein L34





- Molecule 51: 50S ribosomal protein L35



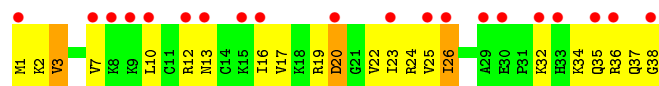
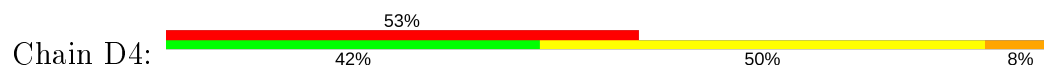
- Molecule 51: 50S ribosomal protein L35



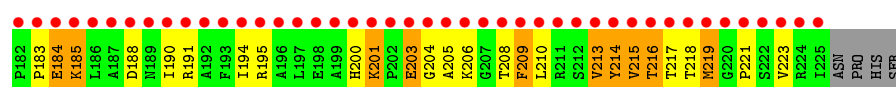
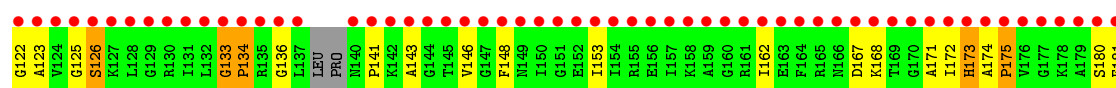
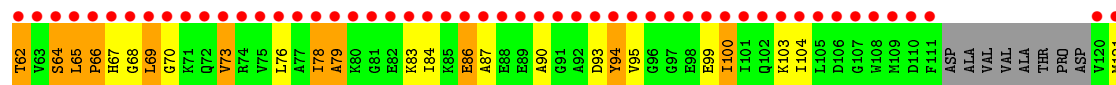
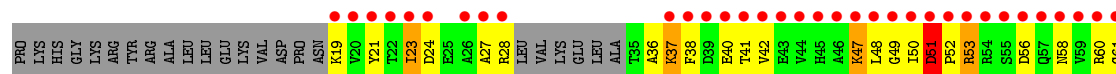
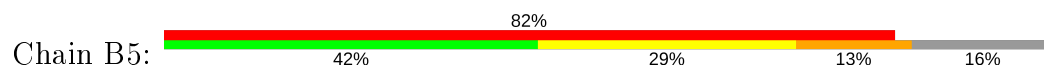
- Molecule 52: 50S ribosomal protein L36



- Molecule 52: 50S ribosomal protein L36



- Molecule 53: 50S ribosomal protein L1



## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 21 21 21  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 210.21Å 433.03Å 619.20Å<br>90.00° 90.00° 90.00°             | Depositor        |
| Resolution (Å)  | 39.97 – 2.90<br>39.97 – 2.90                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 94.9 (39.97-2.90)<br>94.9 (39.97-2.90)                      | Depositor<br>EDS |
| $R_{merge}$   | 0.12  | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.40 (at 2.90Å)   | Xtriage          |
| Refinement program  | PHENIX (phenix.refine: 1.8.1_1168)                          | Depositor        |
| R, $R_{free}$   | 0.220 , 0.264<br>0.225 , 0.269                              | Depositor<br>DCC |
| $R_{free}$ test set   | 4701 reflections (0.40%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 44.0  | Xtriage          |
| Anisotropy  | 0.529   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.27 , 51.6   | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$ | Xtriage          |
| Estimated twinning fraction   | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation  | 0.91  | EDS              |
| Total number of atoms   | 288276  | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 62.0  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.55% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN, DOL

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    | 0.46         | 0/36944     | 0.92        | 22/57632 (0.0%) |
| 1   | CA    | 0.39         | 0/36966     | 0.86        | 4/57666 (0.0%)  |
| 2   | AB    | 0.36         | 0/1736      | 0.58        | 0/2338          |
| 2   | CB    | 0.32         | 0/1736      | 0.53        | 0/2338          |
| 3   | AC    | 0.35         | 0/1652      | 0.57        | 0/2225          |
| 3   | CC    | 0.31         | 0/1652      | 0.51        | 0/2225          |
| 4   | AD    | 0.36         | 0/1665      | 0.61        | 0/2227          |
| 4   | CD    | 0.39         | 0/1665      | 0.61        | 0/2227          |
| 5   | AE    | 0.38         | 0/1119      | 0.66        | 0/1504          |
| 5   | CE    | 0.37         | 0/1119      | 0.65        | 0/1504          |
| 6   | AF    | 0.39         | 0/836       | 0.60        | 0/1128          |
| 6   | CF    | 0.33         | 0/836       | 0.58        | 0/1128          |
| 7   | AG    | 0.34         | 0/1196      | 0.52        | 0/1602          |
| 7   | CG    | 0.31         | 0/1196      | 0.51        | 0/1602          |
| 8   | AH    | 0.38         | 0/989       | 0.57        | 0/1326          |
| 8   | CH    | 0.31         | 0/989       | 0.52        | 0/1326          |
| 9   | AI    | 0.33         | 0/1034      | 0.58        | 0/1375          |
| 9   | CI    | 0.31         | 0/1034      | 0.55        | 0/1375          |
| 10  | AJ    | 0.36         | 0/797       | 0.59        | 0/1077          |
| 10  | CJ    | 0.31         | 0/797       | 0.52        | 0/1077          |
| 11  | AK    | 0.36         | 0/893       | 0.67        | 1/1205 (0.1%)   |
| 11  | CK    | 0.32         | 0/893       | 0.55        | 0/1205          |
| 12  | AL    | 0.41         | 0/969       | 0.65        | 0/1300          |
| 12  | CL    | 0.37         | 0/969       | 0.63        | 0/1300          |
| 13  | AM    | 0.36         | 0/893       | 0.59        | 0/1193          |
| 13  | CM    | 0.32         | 0/893       | 0.52        | 0/1193          |
| 14  | AN    | 0.36         | 0/785       | 0.58        | 0/1043          |
| 14  | CN    | 0.30         | 0/785       | 0.50        | 0/1043          |
| 15  | AO    | 0.36         | 0/718       | 0.58        | 0/959           |
| 15  | CO    | 0.32         | 0/718       | 0.50        | 0/959           |
| 16  | AP    | 0.38         | 0/659       | 0.69        | 1/884 (0.1%)    |
| 16  | CP    | 0.32         | 0/659       | 0.55        | 0/884           |

| Mol | Chain | Bond lengths |                 | Bond angles |                   |
|-----|-------|--------------|-----------------|-------------|-------------------|
|     |       | RMSZ         | # Z  >5         | RMSZ        | # Z  >5           |
| 17  | AQ    | 0.41         | 0/658           | 0.63        | 0/881             |
| 17  | CQ    | 0.33         | 0/658           | 0.54        | 0/881             |
| 18  | AR    | 0.35         | 0/463           | 0.57        | 0/621             |
| 18  | CR    | 0.33         | 0/463           | 0.52        | 0/621             |
| 19  | AS    | 0.36         | 0/653           | 0.53        | 0/877             |
| 19  | CS    | 0.32         | 0/653           | 0.56        | 0/877             |
| 20  | AT    | 0.36         | 0/671           | 0.58        | 0/888             |
| 20  | CT    | 0.30         | 0/671           | 0.54        | 0/888             |
| 21  | AU    | 0.45         | 0/431           | 0.63        | 0/570             |
| 21  | CU    | 0.42         | 0/431           | 0.62        | 0/570             |
| 22  | BA    | 0.84         | 18/69659 (0.0%) | 1.25        | 413/108672 (0.4%) |
| 22  | DA    | 0.37         | 0/69659         | 0.85        | 11/108672 (0.0%)  |
| 23  | BB    | 0.73         | 0/2850          | 1.17        | 11/4444 (0.2%)    |
| 23  | DB    | 0.32         | 0/2828          | 0.80        | 0/4410            |
| 24  | BC    | 0.50         | 0/2122          | 0.70        | 0/2852            |
| 24  | DC    | 0.33         | 0/2122          | 0.56        | 0/2852            |
| 25  | BD    | 0.58         | 0/1586          | 0.75        | 1/2134 (0.0%)     |
| 25  | DD    | 0.31         | 0/1586          | 0.55        | 0/2134            |
| 26  | BE    | 0.50         | 0/1571          | 0.67        | 0/2113            |
| 26  | DE    | 0.31         | 0/1571          | 0.53        | 0/2113            |
| 27  | BF    | 0.40         | 0/1435          | 0.61        | 0/1926            |
| 27  | DF    | 0.29         | 0/1435          | 0.48        | 0/1926            |
| 28  | BG    | 0.40         | 0/1343          | 0.60        | 0/1816            |
| 28  | DG    | 0.30         | 0/1343          | 0.48        | 0/1816            |
| 29  | BH    | 0.36         | 0/1121          | 0.66        | 1/1515 (0.1%)     |
| 29  | DH    | 0.35         | 0/1121          | 0.56        | 0/1515            |
| 30  | BI    | 0.35         | 0/1046          | 0.55        | 0/1410            |
| 30  | DI    | 0.35         | 0/1046          | 0.53        | 0/1410            |
| 31  | BJ    | 0.61         | 0/1152          | 0.73        | 0/1551            |
| 31  | DJ    | 0.31         | 0/1152          | 0.54        | 0/1551            |
| 32  | BK    | 0.61         | 0/948           | 0.75        | 0/1268            |
| 32  | DK    | 0.34         | 0/948           | 0.55        | 0/1268            |
| 33  | BL    | 0.55         | 0/1054          | 0.74        | 0/1403            |
| 33  | DL    | 0.31         | 0/1054          | 0.53        | 0/1403            |
| 34  | BM    | 0.58         | 0/1093          | 0.73        | 0/1460            |
| 34  | DM    | 0.30         | 0/1093          | 0.50        | 0/1460            |
| 35  | BN    | 0.62         | 0/974           | 0.79        | 0/1301            |
| 35  | DN    | 0.33         | 0/974           | 0.58        | 1/1301 (0.1%)     |
| 36  | BO    | 0.48         | 0/902           | 0.64        | 0/1209            |
| 36  | DO    | 0.29         | 0/902           | 0.47        | 0/1209            |
| 37  | BP    | 0.55         | 0/929           | 0.75        | 3/1242 (0.2%)     |
| 37  | DP    | 0.32         | 0/929           | 0.51        | 0/1242            |
| 38  | BQ    | 0.67         | 0/960           | 0.78        | 0/1278            |



| Mol | Chain | Bond lengths |                  | Bond angles |                   |
|-----|-------|--------------|------------------|-------------|-------------------|
|     |       | RMSZ         | # Z  >5          | RMSZ        | # Z  >5           |
| 38  | DQ    | 0.33         | 0/960            | 0.50        | 0/1278            |
| 39  | BR    | 0.64         | 0/829            | 0.84        | 0/1107            |
| 39  | DR    | 0.30         | 0/829            | 0.53        | 0/1107            |
| 40  | BS    | 0.69         | 0/864            | 0.81        | 0/1156            |
| 40  | DS    | 0.32         | 0/864            | 0.54        | 0/1156            |
| 41  | BT    | 0.46         | 0/745            | 0.69        | 0/994             |
| 41  | DT    | 0.31         | 0/745            | 0.51        | 0/994             |
| 42  | BU    | 0.47         | 0/788            | 0.66        | 0/1051            |
| 42  | DU    | 0.34         | 0/788            | 0.56        | 0/1051            |
| 43  | BV    | 0.51         | 0/766            | 0.68        | 0/1025            |
| 43  | DV    | 0.28         | 0/766            | 0.44        | 0/1025            |
| 44  | BW    | 0.60         | 0/587            | 0.74        | 0/776             |
| 44  | DW    | 0.30         | 0/576            | 0.50        | 0/762             |
| 45  | BX    | 0.44         | 0/635            | 0.66        | 0/848             |
| 45  | DX    | 0.33         | 0/635            | 0.55        | 0/848             |
| 46  | BY    | 0.44         | 0/510            | 0.71        | 0/677             |
| 46  | DY    | 0.29         | 0/510            | 0.53        | 0/677             |
| 47  | BZ    | 0.55         | 0/453            | 0.69        | 0/605             |
| 47  | DZ    | 0.31         | 0/453            | 0.51        | 0/605             |
| 48  | B0    | 0.61         | 0/450            | 0.77        | 0/599             |
| 48  | D0    | 0.33         | 0/450            | 0.54        | 0/599             |
| 49  | B1    | 0.48         | 0/417            | 0.62        | 0/554             |
| 49  | D1    | 0.31         | 0/417            | 0.50        | 0/554             |
| 50  | B2    | 0.62         | 0/380            | 0.81        | 0/498             |
| 50  | D2    | 0.34         | 0/380            | 0.55        | 0/498             |
| 51  | B3    | 0.57         | 0/513            | 0.69        | 0/676             |
| 51  | D3    | 0.29         | 0/513            | 0.49        | 0/676             |
| 52  | B4    | 0.57         | 0/303            | 0.70        | 0/397             |
| 52  | D4    | 0.30         | 0/303            | 0.54        | 0/397             |
| 53  | B5    | 0.32         | 0/1145           | 0.50        | 0/1556            |
| All | All   | 0.54         | 18/310626 (0.0%) | 0.92        | 469/464366 (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 |
|-----|-------|---------------------|---------------------|
| 4   | CD    | 0                   | 1                   |
| 5   | AE    | 0                   | 1                   |
| 5   | CE    | 0                   | 1                   |
| 6   | CF    | 0                   | 1                   |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 11  | AK    | 0                   | 1                   |
| 12  | CL    | 0                   | 1                   |
| 25  | BD    | 0                   | 1                   |
| 25  | DD    | 0                   | 1                   |
| All | All   | 0                   | 8                   |

All (18) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|--------|-------------|----------|
| 22  | BA    | 1142 | A    | N9-C4 | -11.42 | 1.31        | 1.37     |
| 22  | BA    | 984  | A    | N9-C4 | -10.72 | 1.31        | 1.37     |
| 22  | BA    | 1936 | A    | N9-C4 | -9.94  | 1.31        | 1.37     |
| 22  | BA    | 528  | A    | N9-C4 | -8.18  | 1.32        | 1.37     |
| 22  | BA    | 783  | A    | N9-C4 | -6.66  | 1.33        | 1.37     |
| 22  | BA    | 561  | G    | N9-C4 | -6.57  | 1.32        | 1.38     |
| 22  | BA    | 984  | A    | N3-C4 | -6.25  | 1.31        | 1.34     |
| 22  | BA    | 528  | A    | N3-C4 | -6.13  | 1.31        | 1.34     |
| 22  | BA    | 571  | U    | N1-C2 | -5.70  | 1.33        | 1.38     |
| 22  | BA    | 528  | A    | N7-C5 | -5.56  | 1.35        | 1.39     |
| 22  | BA    | 1787 | A    | N9-C4 | -5.50  | 1.34        | 1.37     |
| 22  | BA    | 528  | A    | C5-C6 | -5.49  | 1.36        | 1.41     |
| 22  | BA    | 2241 | A    | N9-C4 | -5.44  | 1.34        | 1.37     |
| 22  | BA    | 675  | A    | N9-C4 | -5.21  | 1.34        | 1.37     |
| 22  | BA    | 974  | G    | N9-C8 | 5.21   | 1.41        | 1.37     |
| 22  | BA    | 802  | A    | N7-C5 | -5.10  | 1.36        | 1.39     |
| 22  | BA    | 2623 | G    | N3-C4 | -5.01  | 1.31        | 1.35     |
| 22  | BA    | 2274 | A    | N9-C4 | -5.01  | 1.34        | 1.37     |

All (469) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms    | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 22  | BA    | 984  | A    | C2-N3-C4 | -12.81 | 104.20      | 110.60   |
| 22  | BA    | 974  | G    | C4-C5-N7 | 12.41  | 115.76      | 110.80   |
| 22  | BA    | 1142 | A    | C2-N3-C4 | -11.77 | 104.72      | 110.60   |
| 22  | BA    | 1936 | A    | C2-N3-C4 | -11.57 | 104.81      | 110.60   |
| 22  | BA    | 974  | G    | C5-C6-O6 | -11.27 | 121.84      | 128.60   |
| 22  | BA    | 984  | A    | N3-C4-N9 | -10.86 | 118.71      | 127.40   |
| 25  | BD    | 151  | THR  | C-N-CD   | -10.79 | 96.87       | 120.60   |
| 22  | BA    | 974  | G    | C5-N7-C8 | -10.53 | 99.04       | 104.30   |
| 22  | BA    | 528  | A    | C2-N3-C4 | -10.43 | 105.39      | 110.60   |
| 22  | BA    | 1997 | C    | C6-N1-C2 | 10.29  | 124.42      | 120.30   |
| 22  | BA    | 752  | A    | C5-N7-C8 | -9.95  | 98.92       | 103.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 22  | BA    | 2286 | G    | N3-C4-C5   | 9.86  | 133.53      | 128.60   |
| 22  | BA    | 984  | A    | N3-C4-C5   | 9.84  | 133.69      | 126.80   |
| 22  | BA    | 1936 | A    | N1-C6-N6   | 9.82  | 124.49      | 118.60   |
| 22  | BA    | 1783 | A    | O5'-P-OP2  | -9.21 | 97.41       | 105.70   |
| 22  | BA    | 752  | A    | N7-C8-N9   | 8.88  | 118.24      | 113.80   |
| 22  | BA    | 783  | A    | C2-N3-C4   | -8.83 | 106.18      | 110.60   |
| 22  | BA    | 1142 | A    | N3-C4-C5   | 8.78  | 132.94      | 126.80   |
| 22  | BA    | 784  | G    | O4'-C1'-N9 | -8.69 | 101.25      | 108.20   |
| 22  | BA    | 1779 | U    | C5-C4-O4   | 8.68  | 131.11      | 125.90   |
| 22  | BA    | 528  | A    | N1-C6-N6   | 8.60  | 123.76      | 118.60   |
| 22  | BA    | 586  | A    | O5'-P-OP1  | -8.52 | 98.03       | 105.70   |
| 22  | BA    | 561  | G    | N3-C4-C5   | 8.48  | 132.84      | 128.60   |
| 22  | BA    | 2263 | C    | C6-N1-C2   | 8.34  | 123.64      | 120.30   |
| 22  | BA    | 1985 | C    | C6-N1-C2   | 8.26  | 123.60      | 120.30   |
| 16  | AP    | 51   | ARG  | NE-CZ-NH1  | 8.25  | 124.42      | 120.30   |
| 22  | BA    | 974  | G    | N1-C6-O6   | 8.20  | 124.82      | 119.90   |
| 22  | BA    | 2030 | A    | C5-C6-N1   | -8.20 | 113.60      | 117.70   |
| 22  | BA    | 1936 | A    | N3-C4-C5   | 8.16  | 132.51      | 126.80   |
| 22  | BA    | 824  | U    | O5'-P-OP2  | -8.13 | 98.38       | 105.70   |
| 22  | BA    | 783  | A    | C5-N7-C8   | -8.12 | 99.84       | 103.90   |
| 22  | BA    | 532  | A    | O5'-P-OP1  | -8.11 | 98.40       | 105.70   |
| 37  | BP    | 103  | ARG  | NE-CZ-NH1  | 8.00  | 124.30      | 120.30   |
| 22  | BA    | 528  | A    | C5-C6-N1   | -7.97 | 113.71      | 117.70   |
| 22  | BA    | 691  | C    | C6-N1-C2   | 7.96  | 123.48      | 120.30   |
| 22  | BA    | 555  | G    | O5'-P-OP1  | -7.86 | 98.62       | 105.70   |
| 22  | BA    | 850  | U    | O5'-P-OP1  | -7.85 | 98.64       | 105.70   |
| 22  | BA    | 2250 | G    | C5-N7-C8   | -7.79 | 100.41      | 104.30   |
| 22  | BA    | 1795 | C    | O5'-P-OP1  | -7.74 | 98.74       | 105.70   |
| 22  | BA    | 752  | A    | C4-C5-N7   | 7.72  | 114.56      | 110.70   |
| 22  | BA    | 1645 | G    | C4-C5-N7   | 7.72  | 113.89      | 110.80   |
| 22  | BA    | 2359 | C    | O5'-P-OP2  | 7.72  | 119.97      | 110.70   |
| 22  | BA    | 1997 | C    | N3-C4-C5   | 7.71  | 124.98      | 121.90   |
| 22  | BA    | 1142 | A    | N3-C4-N9   | -7.68 | 121.25      | 127.40   |
| 22  | BA    | 2606 | C    | N3-C4-C5   | 7.66  | 124.97      | 121.90   |
| 22  | BA    | 2705 | A    | N1-C6-N6   | 7.62  | 123.17      | 118.60   |
| 22  | BA    | 1779 | U    | N3-C4-O4   | -7.61 | 114.07      | 119.40   |
| 22  | BA    | 974  | G    | C6-C5-N7   | -7.56 | 125.86      | 130.40   |
| 22  | BA    | 2286 | G    | C2-N3-C4   | -7.52 | 108.14      | 111.90   |
| 22  | BA    | 2606 | C    | C6-N1-C2   | 7.50  | 123.30      | 120.30   |
| 22  | BA    | 1658 | C    | C5-C4-N4   | -7.50 | 114.95      | 120.20   |
| 22  | BA    | 1658 | C    | C6-N1-C2   | 7.47  | 123.29      | 120.30   |
| 22  | BA    | 974  | G    | N7-C8-N9   | 7.43  | 116.82      | 113.10   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 22  | BA    | 757  | G    | C8-N9-C4   | 7.40  | 109.36      | 106.40   |
| 22  | BA    | 528  | A    | C5-N7-C8   | -7.39 | 100.20      | 103.90   |
| 22  | BA    | 1663 | G    | C8-N9-C4   | 7.37  | 109.35      | 106.40   |
| 35  | DN    | 71   | ARG  | NE-CZ-NH2  | 7.37  | 123.98      | 120.30   |
| 22  | BA    | 1266 | G    | O5'-P-OP1  | -7.30 | 99.13       | 105.70   |
| 22  | BA    | 1788 | C    | C5-C4-N4   | -7.29 | 115.10      | 120.20   |
| 22  | BA    | 2250 | G    | C4-C5-N7   | 7.27  | 113.71      | 110.80   |
| 22  | BA    | 752  | A    | N1-C6-N6   | 7.24  | 122.94      | 118.60   |
| 22  | BA    | 783  | A    | N1-C6-N6   | 7.21  | 122.93      | 118.60   |
| 22  | BA    | 1142 | A    | C5-N7-C8   | -7.21 | 100.29      | 103.90   |
| 22  | BA    | 783  | A    | C4-C5-N7   | 7.20  | 114.30      | 110.70   |
| 22  | BA    | 1764 | C    | C6-N1-C2   | 7.18  | 123.17      | 120.30   |
| 22  | BA    | 837  | C    | N1-C2-O2   | -7.17 | 114.60      | 118.90   |
| 22  | BA    | 2585 | U    | O4'-C1'-N1 | 7.16  | 113.93      | 108.20   |
| 22  | BA    | 1617 | C    | O5'-P-OP2  | -7.16 | 99.26       | 105.70   |
| 22  | BA    | 957  | C    | C6-N1-C2   | 7.13  | 123.15      | 120.30   |
| 22  | BA    | 752  | A    | C6-C5-N7   | -7.13 | 127.31      | 132.30   |
| 22  | BA    | 1045 | C    | C6-N1-C2   | 7.12  | 123.15      | 120.30   |
| 22  | BA    | 2045 | C    | C6-N1-C2   | 7.09  | 123.14      | 120.30   |
| 22  | BA    | 794  | A    | N1-C6-N6   | 7.07  | 122.84      | 118.60   |
| 22  | BA    | 1663 | G    | C2-N3-C4   | -7.06 | 108.37      | 111.90   |
| 22  | BA    | 704  | G    | O4'-C1'-N9 | 7.05  | 113.84      | 108.20   |
| 22  | BA    | 2286 | G    | N3-C4-N9   | -7.00 | 121.80      | 126.00   |
| 22  | BA    | 783  | A    | N3-C4-C5   | 6.95  | 131.66      | 126.80   |
| 22  | BA    | 784  | G    | P-O3'-C3'  | 6.93  | 128.01      | 119.70   |
| 22  | BA    | 1645 | G    | N3-C2-N2   | 6.92  | 124.74      | 119.90   |
| 22  | BA    | 2325 | G    | O5'-P-OP2  | -6.91 | 99.48       | 105.70   |
| 22  | BA    | 2715 | C    | N3-C2-O2   | -6.91 | 117.07      | 121.90   |
| 22  | BA    | 528  | A    | N3-C4-C5   | 6.89  | 131.62      | 126.80   |
| 22  | BA    | 574  | A    | N1-C6-N6   | -6.87 | 114.48      | 118.60   |
| 22  | BA    | 1646 | C    | C6-N1-C2   | 6.83  | 123.03      | 120.30   |
| 22  | BA    | 2009 | A    | O5'-P-OP2  | -6.83 | 99.56       | 105.70   |
| 22  | BA    | 2035 | G    | O5'-P-OP2  | -6.82 | 99.56       | 105.70   |
| 22  | BA    | 984  | A    | C5-C6-N1   | -6.81 | 114.29      | 117.70   |
| 22  | BA    | 1900 | A    | O5'-P-OP1  | -6.81 | 99.57       | 105.70   |
| 22  | BA    | 672  | C    | C6-N1-C2   | 6.80  | 123.02      | 120.30   |
| 22  | BA    | 2326 | C    | C6-N1-C2   | -6.79 | 117.59      | 120.30   |
| 22  | BA    | 1157 | G    | O5'-P-OP2  | -6.76 | 99.62       | 105.70   |
| 22  | BA    | 2639 | A    | C5-C6-N6   | -6.76 | 118.29      | 123.70   |
| 22  | BA    | 2013 | A    | O5'-P-OP2  | -6.75 | 99.63       | 105.70   |
| 22  | BA    | 2817 | U    | C6-N1-C2   | 6.71  | 125.03      | 121.00   |
| 22  | BA    | 1649 | G    | C8-N9-C4   | -6.70 | 103.72      | 106.40   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 22  | BA    | 2874 | C    | N3-C4-C5   | 6.69  | 124.58      | 121.90   |
| 22  | BA    | 1779 | U    | C5-C6-N1   | -6.68 | 119.36      | 122.70   |
| 22  | BA    | 2814 | A    | N1-C6-N6   | 6.67  | 122.60      | 118.60   |
| 23  | BB    | 79   | G    | C5-C6-O6   | -6.65 | 124.61      | 128.60   |
| 22  | BA    | 1790 | C    | N3-C4-C5   | 6.62  | 124.55      | 121.90   |
| 22  | BA    | 1478 | G    | N3-C2-N2   | -6.62 | 115.27      | 119.90   |
| 22  | BA    | 664  | G    | O5'-P-OP2  | -6.58 | 99.78       | 105.70   |
| 22  | BA    | 2518 | A    | O4'-C1'-N9 | -6.58 | 102.94      | 108.20   |
| 22  | BA    | 2580 | U    | OP2-P-O3'  | 6.56  | 119.64      | 105.20   |
| 22  | BA    | 395  | U    | O4'-C1'-N1 | 6.56  | 113.45      | 108.20   |
| 22  | BA    | 835  | C    | C6-N1-C2   | 6.56  | 122.92      | 120.30   |
| 22  | BA    | 2033 | A    | N1-C6-N6   | -6.55 | 114.67      | 118.60   |
| 22  | BA    | 2612 | C    | N3-C4-C5   | 6.54  | 124.52      | 121.90   |
| 22  | BA    | 1606 | C    | P-O3'-C3'  | 6.53  | 127.54      | 119.70   |
| 22  | BA    | 1452 | G    | C5-N7-C8   | -6.53 | 101.04      | 104.30   |
| 22  | BA    | 2463 | C    | O5'-P-OP1  | -6.51 | 99.84       | 105.70   |
| 22  | BA    | 1478 | G    | N1-C6-O6   | 6.50  | 123.80      | 119.90   |
| 22  | BA    | 2820 | A    | N1-C6-N6   | 6.50  | 122.50      | 118.60   |
| 22  | BA    | 2607 | G    | C5-C6-O6   | -6.49 | 124.71      | 128.60   |
| 22  | DA    | 2427 | C    | C6-N1-C2   | -6.49 | 117.70      | 120.30   |
| 22  | BA    | 1640 | A    | N1-C6-N6   | -6.48 | 114.71      | 118.60   |
| 22  | BA    | 2716 | C    | O5'-P-OP2  | -6.47 | 99.87       | 105.70   |
| 1   | AA    | 1530 | G    | N3-C4-C5   | 6.46  | 131.83      | 128.60   |
| 22  | BA    | 1663 | G    | N3-C4-C5   | 6.42  | 131.81      | 128.60   |
| 22  | BA    | 1340 | U    | C5-C4-O4   | 6.41  | 129.75      | 125.90   |
| 22  | BA    | 1134 | A    | O5'-P-OP1  | -6.40 | 99.94       | 105.70   |
| 22  | BA    | 2715 | C    | N1-C2-O2   | 6.39  | 122.73      | 118.90   |
| 22  | BA    | 1549 | A    | N1-C6-N6   | 6.38  | 122.43      | 118.60   |
| 22  | BA    | 938  | G    | C4-N9-C1'  | -6.38 | 118.21      | 126.50   |
| 22  | BA    | 2030 | A    | C5-C6-N6   | 6.38  | 128.80      | 123.70   |
| 22  | BA    | 2250 | G    | N3-C4-C5   | 6.37  | 131.79      | 128.60   |
| 22  | BA    | 1645 | G    | C6-C5-N7   | -6.36 | 126.58      | 130.40   |
| 22  | BA    | 748  | G    | O4'-C1'-N9 | 6.35  | 113.28      | 108.20   |
| 22  | BA    | 2645 | G    | O4'-C1'-N9 | 6.35  | 113.28      | 108.20   |
| 22  | BA    | 1138 | G    | C8-N9-C4   | -6.35 | 103.86      | 106.40   |
| 11  | AK    | 128  | ARG  | NE-CZ-NH1  | 6.34  | 123.47      | 120.30   |
| 22  | BA    | 2825 | G    | N3-C4-C5   | -6.34 | 125.43      | 128.60   |
| 22  | BA    | 2499 | C    | N1-C2-O2   | -6.34 | 115.10      | 118.90   |
| 22  | DA    | 691  | C    | C6-N1-C2   | -6.33 | 117.77      | 120.30   |
| 22  | BA    | 2250 | G    | C2-N3-C4   | -6.32 | 108.74      | 111.90   |
| 22  | BA    | 967  | U    | N3-C4-O4   | -6.30 | 114.99      | 119.40   |
| 22  | BA    | 1762 | A    | N1-C6-N6   | 6.30  | 122.38      | 118.60   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 22  | BA    | 529  | A    | C8-N9-C4   | 6.29  | 108.32      | 105.80   |
| 22  | BA    | 1779 | U    | N3-C2-O2   | -6.29 | 117.80      | 122.20   |
| 22  | BA    | 560  | C    | C6-N1-C2   | 6.24  | 122.80      | 120.30   |
| 23  | BB    | 99   | A    | C2-N3-C4   | -6.24 | 107.48      | 110.60   |
| 22  | BA    | 1652 | A    | C8-N9-C4   | -6.23 | 103.31      | 105.80   |
| 22  | BA    | 2076 | U    | C5-C4-O4   | 6.23  | 129.64      | 125.90   |
| 22  | BA    | 1147 | A    | O5'-P-OP2  | -6.22 | 100.10      | 105.70   |
| 1   | AA    | 578  | C    | O5'-P-OP1  | -6.22 | 100.11      | 105.70   |
| 1   | AA    | 742  | G    | C8-N9-C4   | 6.20  | 108.88      | 106.40   |
| 22  | BA    | 1550 | C    | N1-C2-O2   | -6.19 | 115.18      | 118.90   |
| 22  | BA    | 1620 | G    | C2-N3-C4   | -6.16 | 108.82      | 111.90   |
| 22  | BA    | 2010 | G    | C4-C5-N7   | -6.16 | 108.33      | 110.80   |
| 22  | BA    | 528  | A    | C4-C5-N7   | 6.15  | 113.78      | 110.70   |
| 1   | AA    | 1514 | G    | C5-C6-O6   | -6.14 | 124.91      | 128.60   |
| 22  | BA    | 1296 | G    | N3-C2-N2   | 6.14  | 124.20      | 119.90   |
| 22  | BA    | 2799 | A    | N1-C6-N6   | 6.12  | 122.27      | 118.60   |
| 22  | BA    | 2874 | C    | C5-C4-N4   | -6.12 | 115.92      | 120.20   |
| 22  | BA    | 752  | A    | C8-N9-C4   | -6.12 | 103.35      | 105.80   |
| 22  | BA    | 675  | A    | C8-N9-C4   | 6.11  | 108.24      | 105.80   |
| 22  | BA    | 2011 | U    | N3-C2-O2   | 6.11  | 126.47      | 122.20   |
| 22  | BA    | 1937 | A    | O4'-C1'-N9 | 6.11  | 113.08      | 108.20   |
| 22  | BA    | 2639 | A    | N1-C6-N6   | 6.11  | 122.26      | 118.60   |
| 22  | BA    | 967  | U    | C5-C4-O4   | 6.09  | 129.56      | 125.90   |
| 22  | BA    | 2825 | G    | C4-N9-C1'  | 6.09  | 134.41      | 126.50   |
| 22  | BA    | 1223 | G    | N1-C6-O6   | -6.08 | 116.25      | 119.90   |
| 22  | BA    | 691  | C    | N3-C4-C5   | 6.07  | 124.33      | 121.90   |
| 22  | BA    | 2490 | G    | N3-C4-N9   | 6.07  | 129.64      | 126.00   |
| 22  | BA    | 1936 | A    | N3-C4-N9   | -6.05 | 122.56      | 127.40   |
| 1   | AA    | 365  | U    | C2-N1-C1'  | -6.04 | 110.45      | 117.70   |
| 22  | BA    | 2283 | C    | N1-C2-O2   | -6.04 | 115.28      | 118.90   |
| 22  | BA    | 2837 | A    | O5'-P-OP1  | -6.04 | 100.26      | 105.70   |
| 22  | DA    | 1313 | U    | C2-N1-C1'  | 6.04  | 124.95      | 117.70   |
| 22  | BA    | 243  | U    | C5-C4-O4   | -6.03 | 122.28      | 125.90   |
| 22  | BA    | 2505 | G    | C8-N9-C4   | -6.03 | 103.99      | 106.40   |
| 22  | BA    | 1645 | G    | N1-C2-N2   | -6.02 | 110.79      | 116.20   |
| 22  | BA    | 752  | A    | O4'-C1'-N9 | 6.01  | 113.01      | 108.20   |
| 22  | BA    | 1812 | U    | O5'-P-OP2  | -6.01 | 100.29      | 105.70   |
| 22  | BA    | 2705 | A    | C5-C6-N6   | -5.99 | 118.91      | 123.70   |
| 22  | BA    | 2355 | G    | N3-C2-N2   | -5.97 | 115.72      | 119.90   |
| 22  | BA    | 2536 | G    | C8-N9-C4   | 5.97  | 108.79      | 106.40   |
| 22  | BA    | 1936 | A    | C5-N7-C8   | -5.96 | 100.92      | 103.90   |
| 22  | BA    | 2811 | G    | O5'-P-OP2  | -5.95 | 100.35      | 105.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 22  | BA    | 1997 | C    | C2-N1-C1'  | -5.94 | 112.26      | 118.80   |
| 22  | BA    | 1229 | C    | N1-C2-O2   | -5.94 | 115.33      | 118.90   |
| 22  | BA    | 1645 | G    | N9-C4-C5   | -5.94 | 103.02      | 105.40   |
| 22  | BA    | 1134 | A    | OP1-P-OP2  | 5.93  | 128.50      | 119.60   |
| 22  | BA    | 2827 | C    | C5-C4-N4   | -5.92 | 116.05      | 120.20   |
| 22  | BA    | 2283 | C    | C6-N1-C2   | 5.91  | 122.67      | 120.30   |
| 22  | BA    | 512  | G    | O4'-C1'-N9 | 5.91  | 112.93      | 108.20   |
| 22  | BA    | 561  | G    | C5-C6-O6   | -5.90 | 125.06      | 128.60   |
| 22  | BA    | 758  | C    | C2-N3-C4   | -5.89 | 116.95      | 119.90   |
| 22  | BA    | 554  | U    | O5'-P-OP1  | 5.89  | 117.77      | 110.70   |
| 22  | BA    | 535  | G    | N3-C2-N2   | 5.89  | 124.02      | 119.90   |
| 22  | BA    | 2083 | G    | N3-C4-C5   | 5.87  | 131.54      | 128.60   |
| 22  | BA    | 2480 | C    | N1-C2-O2   | -5.86 | 115.38      | 118.90   |
| 1   | AA    | 819  | A    | O5'-P-OP1  | -5.86 | 100.43      | 105.70   |
| 22  | BA    | 2490 | G    | O5'-P-OP2  | -5.85 | 100.43      | 105.70   |
| 22  | BA    | 1288 | G    | O4'-C1'-N9 | 5.85  | 112.88      | 108.20   |
| 23  | BB    | 75   | G    | O5'-P-OP2  | 5.85  | 117.72      | 110.70   |
| 22  | BA    | 1706 | C    | C6-N1-C2   | 5.84  | 122.64      | 120.30   |
| 22  | BA    | 489  | G    | C5-C6-O6   | -5.84 | 125.10      | 128.60   |
| 1   | AA    | 4    | U    | C2-N1-C1'  | 5.84  | 124.71      | 117.70   |
| 22  | BA    | 2385 | C    | C6-N1-C2   | 5.83  | 122.63      | 120.30   |
| 22  | BA    | 711  | G    | C4-N9-C1'  | -5.82 | 118.93      | 126.50   |
| 22  | BA    | 2715 | C    | O5'-P-OP2  | -5.82 | 100.46      | 105.70   |
| 1   | CA    | 1397 | C    | C6-N1-C2   | -5.81 | 117.97      | 120.30   |
| 23  | BB    | 83   | G    | O5'-P-OP2  | -5.80 | 100.48      | 105.70   |
| 22  | BA    | 454  | A    | O5'-P-OP2  | -5.80 | 100.48      | 105.70   |
| 22  | BA    | 1444 | G    | O5'-P-OP2  | -5.80 | 100.48      | 105.70   |
| 22  | BA    | 2534 | A    | N1-C6-N6   | 5.80  | 122.08      | 118.60   |
| 22  | BA    | 2083 | G    | N1-C6-O6   | 5.80  | 123.38      | 119.90   |
| 22  | BA    | 2419 | U    | C2-N1-C1'  | -5.79 | 110.75      | 117.70   |
| 22  | BA    | 1763 | G    | N3-C4-C5   | 5.79  | 131.50      | 128.60   |
| 22  | BA    | 561  | G    | N3-C4-N9   | -5.79 | 122.53      | 126.00   |
| 22  | BA    | 956  | G    | N1-C6-O6   | 5.78  | 123.37      | 119.90   |
| 22  | BA    | 535  | G    | OP2-P-O3'  | 5.77  | 117.89      | 105.20   |
| 22  | BA    | 1260 | A    | O5'-P-OP2  | -5.76 | 100.51      | 105.70   |
| 23  | BB    | 26   | C    | C6-N1-C2   | 5.75  | 122.60      | 120.30   |
| 22  | BA    | 2538 | C    | C6-N1-C2   | 5.74  | 122.59      | 120.30   |
| 22  | BA    | 2526 | G    | N3-C4-N9   | -5.73 | 122.56      | 126.00   |
| 22  | BA    | 711  | G    | C8-N9-C1'  | 5.73  | 134.45      | 127.00   |
| 22  | BA    | 2827 | C    | N3-C4-N4   | 5.72  | 122.01      | 118.00   |
| 22  | BA    | 2283 | C    | N3-C2-O2   | 5.72  | 125.90      | 121.90   |
| 22  | BA    | 824  | U    | O5'-P-OP1  | 5.71  | 117.55      | 110.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 22  | BA    | 984  | A    | C8-N9-C1'  | 5.71  | 137.98      | 127.70   |
| 1   | AA    | 971  | G    | O4'-C1'-N9 | 5.70  | 112.76      | 108.20   |
| 22  | BA    | 528  | A    | N3-C4-N9   | -5.70 | 122.84      | 127.40   |
| 22  | BA    | 853  | C    | N1-C2-O2   | -5.70 | 115.48      | 118.90   |
| 22  | BA    | 446  | G    | N9-C4-C5   | -5.69 | 103.12      | 105.40   |
| 22  | BA    | 1295 | C    | N1-C2-O2   | -5.69 | 115.48      | 118.90   |
| 22  | BA    | 1616 | A    | N1-C6-N6   | 5.69  | 122.01      | 118.60   |
| 22  | BA    | 2387 | U    | N3-C2-O2   | -5.69 | 118.22      | 122.20   |
| 22  | BA    | 2840 | C    | O5'-P-OP2  | -5.68 | 100.59      | 105.70   |
| 22  | BA    | 1989 | G    | C5-C6-O6   | -5.68 | 125.19      | 128.60   |
| 22  | BA    | 2276 | G    | O5'-P-OP1  | -5.68 | 100.59      | 105.70   |
| 22  | BA    | 1452 | G    | C4-C5-N7   | 5.67  | 113.07      | 110.80   |
| 22  | BA    | 1997 | C    | C5-C6-N1   | -5.67 | 118.16      | 121.00   |
| 22  | BA    | 1790 | C    | C2-N3-C4   | -5.67 | 117.06      | 119.90   |
| 22  | BA    | 1658 | C    | N3-C4-N4   | 5.67  | 121.97      | 118.00   |
| 1   | AA    | 330  | C    | N3-C4-C5   | 5.65  | 124.16      | 121.90   |
| 22  | BA    | 2608 | G    | N3-C2-N2   | -5.64 | 115.95      | 119.90   |
| 1   | AA    | 188  | C    | C2-N1-C1'  | 5.64  | 125.00      | 118.80   |
| 22  | BA    | 837  | C    | C2-N1-C1'  | -5.64 | 112.60      | 118.80   |
| 22  | BA    | 528  | A    | C6-C5-N7   | -5.63 | 128.36      | 132.30   |
| 22  | BA    | 1645 | G    | N3-C4-N9   | 5.62  | 129.37      | 126.00   |
| 22  | BA    | 2295 | C    | C6-N1-C2   | -5.61 | 118.05      | 120.30   |
| 22  | BA    | 820  | A    | OP2-P-O3'  | 5.61  | 117.53      | 105.20   |
| 22  | BA    | 192  | C    | N1-C2-O2   | -5.60 | 115.54      | 118.90   |
| 22  | BA    | 2492 | U    | O5'-P-OP2  | -5.60 | 100.66      | 105.70   |
| 23  | BB    | 15   | A    | N1-C6-N6   | 5.59  | 121.96      | 118.60   |
| 22  | BA    | 698  | C    | C6-N1-C2   | 5.59  | 122.53      | 120.30   |
| 22  | BA    | 2607 | G    | C6-C5-N7   | -5.58 | 127.05      | 130.40   |
| 22  | BA    | 735  | A    | N1-C6-N6   | 5.58  | 121.95      | 118.60   |
| 22  | BA    | 1692 | U    | N3-C2-O2   | 5.58  | 126.10      | 122.20   |
| 1   | CA    | 4    | U    | C2-N1-C1'  | 5.57  | 124.39      | 117.70   |
| 22  | BA    | 533  | G    | N9-C4-C5   | -5.57 | 103.17      | 105.40   |
| 22  | BA    | 2444 | G    | OP2-P-O3'  | 5.57  | 117.45      | 105.20   |
| 22  | BA    | 1223 | G    | C5-C6-O6   | 5.57  | 131.94      | 128.60   |
| 22  | BA    | 2618 | G    | O5'-P-OP1  | -5.57 | 100.69      | 105.70   |
| 22  | BA    | 1653 | G    | N9-C4-C5   | 5.56  | 107.62      | 105.40   |
| 22  | BA    | 1677 | A    | C6-C5-N7   | -5.56 | 128.41      | 132.30   |
| 22  | BA    | 2494 | G    | C5-C6-O6   | 5.56  | 131.94      | 128.60   |
| 22  | BA    | 2036 | C    | OP2-P-O3'  | 5.56  | 117.43      | 105.20   |
| 22  | BA    | 1472 | C    | C6-N1-C2   | 5.55  | 122.52      | 120.30   |
| 22  | BA    | 2579 | C    | OP1-P-O3'  | 5.55  | 117.42      | 105.20   |
| 22  | BA    | 1681 | G    | C5-C6-O6   | -5.55 | 125.27      | 128.60   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 22  | BA    | 1799 | G    | C8-N9-C4   | 5.55  | 108.62      | 106.40   |
| 22  | BA    | 2418 | A    | O5'-P-OP2  | -5.55 | 100.71      | 105.70   |
| 22  | BA    | 1638 | C    | C6-N1-C2   | 5.55  | 122.52      | 120.30   |
| 22  | BA    | 2076 | U    | N3-C4-O4   | -5.55 | 115.52      | 119.40   |
| 22  | BA    | 2089 | C    | C2-N3-C4   | -5.54 | 117.13      | 119.90   |
| 22  | BA    | 2462 | C    | O5'-P-OP1  | -5.54 | 100.71      | 105.70   |
| 22  | BA    | 1817 | G    | C2-N3-C4   | -5.54 | 109.13      | 111.90   |
| 22  | BA    | 2887 | A    | N1-C6-N6   | 5.54  | 121.92      | 118.60   |
| 22  | BA    | 2490 | G    | N3-C4-C5   | -5.52 | 125.84      | 128.60   |
| 22  | BA    | 2684 | U    | OP2-P-O3'  | 5.51  | 117.33      | 105.20   |
| 22  | BA    | 40   | U    | O5'-P-OP1  | -5.51 | 100.74      | 105.70   |
| 22  | BA    | 765  | C    | O5'-P-OP2  | -5.50 | 100.75      | 105.70   |
| 1   | AA    | 365  | U    | C5-C4-O4   | 5.50  | 129.20      | 125.90   |
| 23  | BB    | 71   | C    | N3-C4-C5   | 5.50  | 124.10      | 121.90   |
| 22  | BA    | 805  | G    | N3-C4-C5   | 5.49  | 131.35      | 128.60   |
| 22  | BA    | 1616 | A    | C4-C5-N7   | 5.49  | 113.44      | 110.70   |
| 22  | BA    | 177  | G    | O4'-C1'-N9 | 5.48  | 112.58      | 108.20   |
| 22  | BA    | 2439 | A    | N1-C6-N6   | 5.48  | 121.89      | 118.60   |
| 22  | BA    | 1138 | G    | N7-C8-N9   | 5.47  | 115.84      | 113.10   |
| 22  | BA    | 1938 | A    | C8-N9-C4   | 5.47  | 107.99      | 105.80   |
| 22  | BA    | 2615 | U    | C5-C4-O4   | -5.46 | 122.62      | 125.90   |
| 1   | AA    | 400  | C    | C6-N1-C2   | 5.46  | 122.48      | 120.30   |
| 22  | BA    | 1761 | C    | O5'-P-OP1  | -5.46 | 100.79      | 105.70   |
| 22  | BA    | 2815 | C    | N1-C2-O2   | -5.46 | 115.63      | 118.90   |
| 22  | BA    | 711  | G    | N3-C4-N9   | -5.45 | 122.73      | 126.00   |
| 22  | BA    | 2351 | G    | O5'-P-OP2  | -5.45 | 100.80      | 105.70   |
| 22  | BA    | 456  | C    | O5'-P-OP2  | -5.44 | 100.81      | 105.70   |
| 22  | BA    | 1804 | C    | N1-C2-O2   | -5.44 | 115.64      | 118.90   |
| 22  | BA    | 2332 | C    | N1-C2-O2   | -5.44 | 115.64      | 118.90   |
| 22  | BA    | 2839 | G    | OP2-P-O3'  | 5.44  | 117.16      | 105.20   |
| 22  | BA    | 1799 | G    | N3-C4-C5   | 5.43  | 131.32      | 128.60   |
| 22  | BA    | 2003 | A    | O5'-P-OP2  | 5.43  | 117.22      | 110.70   |
| 22  | BA    | 1936 | A    | N1-C2-N3   | 5.43  | 132.01      | 129.30   |
| 22  | BA    | 1340 | U    | N3-C4-O4   | -5.43 | 115.60      | 119.40   |
| 22  | BA    | 2072 | C    | C5-C4-N4   | -5.43 | 116.40      | 120.20   |
| 22  | BA    | 995  | C    | O4'-C1'-N1 | -5.43 | 103.86      | 108.20   |
| 22  | BA    | 2275 | C    | C6-N1-C2   | -5.43 | 118.13      | 120.30   |
| 22  | DA    | 793  | A    | C8-N9-C4   | 5.43  | 107.97      | 105.80   |
| 23  | BB    | 55   | U    | N1-C2-O2   | -5.42 | 119.00      | 122.80   |
| 22  | BA    | 938  | G    | C8-N9-C1'  | 5.42  | 134.04      | 127.00   |
| 22  | BA    | 753  | A    | OP1-P-OP2  | 5.41  | 127.72      | 119.60   |
| 1   | AA    | 330  | C    | C6-N1-C2   | 5.41  | 122.46      | 120.30   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 22  | BA    | 1048 | A    | N1-C6-N6   | 5.41  | 121.84      | 118.60   |
| 22  | BA    | 2276 | G    | C5-C6-O6   | 5.41  | 131.84      | 128.60   |
| 22  | DA    | 1246 | A    | N1-C6-N6   | 5.41  | 121.84      | 118.60   |
| 22  | BA    | 532  | A    | OP1-P-OP2  | 5.40  | 127.71      | 119.60   |
| 22  | BA    | 2045 | C    | N3-C4-C5   | 5.40  | 124.06      | 121.90   |
| 22  | BA    | 2503 | A    | C2-N3-C4   | 5.39  | 113.30      | 110.60   |
| 22  | BA    | 560  | C    | N3-C4-C5   | 5.39  | 124.06      | 121.90   |
| 22  | BA    | 1779 | U    | O4'-C1'-N1 | 5.38  | 112.51      | 108.20   |
| 22  | BA    | 2887 | A    | C5-C6-N6   | -5.38 | 119.39      | 123.70   |
| 22  | BA    | 502  | A    | O5'-P-OP1  | -5.38 | 100.86      | 105.70   |
| 22  | BA    | 1326 | U    | N1-C2-O2   | -5.37 | 119.04      | 122.80   |
| 22  | BA    | 1783 | A    | N1-C6-N6   | 5.37  | 121.82      | 118.60   |
| 22  | BA    | 243  | U    | N3-C2-O2   | 5.37  | 125.96      | 122.20   |
| 1   | AA    | 1504 | G    | O4'-C1'-N9 | 5.37  | 112.49      | 108.20   |
| 22  | BA    | 1786 | A    | C2-N3-C4   | 5.36  | 113.28      | 110.60   |
| 22  | BA    | 998  | C    | C6-N1-C2   | -5.36 | 118.16      | 120.30   |
| 37  | BP    | 53   | ARG  | NE-CZ-NH1  | 5.36  | 122.98      | 120.30   |
| 22  | BA    | 1651 | G    | OP1-P-O3'  | 5.35  | 116.98      | 105.20   |
| 22  | BA    | 2420 | C    | N1-C2-O2   | -5.35 | 115.69      | 118.90   |
| 22  | BA    | 836  | G    | C5-C6-O6   | -5.35 | 125.39      | 128.60   |
| 22  | BA    | 2499 | C    | N3-C2-O2   | 5.35  | 125.64      | 121.90   |
| 22  | BA    | 530  | G    | O4'-C1'-N9 | -5.34 | 103.92      | 108.20   |
| 22  | BA    | 974  | G    | O4'-C1'-N9 | 5.34  | 112.47      | 108.20   |
| 22  | BA    | 2211 | A    | P-O3'-C3'  | 5.34  | 126.11      | 119.70   |
| 1   | AA    | 1414 | U    | C2-N1-C1'  | -5.34 | 111.30      | 117.70   |
| 22  | BA    | 1677 | A    | N1-C6-N6   | 5.33  | 121.80      | 118.60   |
| 22  | BA    | 2002 | G    | C5-C6-O6   | -5.33 | 125.41      | 128.60   |
| 22  | BA    | 2813 | A    | N3-C4-C5   | 5.33  | 130.53      | 126.80   |
| 22  | BA    | 1262 | A    | C8-N9-C4   | -5.32 | 103.67      | 105.80   |
| 22  | BA    | 822  | G    | C8-N9-C4   | 5.32  | 108.53      | 106.40   |
| 22  | BA    | 2869 | G    | C5-C6-O6   | -5.32 | 125.41      | 128.60   |
| 22  | BA    | 984  | A    | C4-N9-C1'  | -5.31 | 116.74      | 126.30   |
| 22  | BA    | 2286 | G    | C4-N9-C1'  | -5.31 | 119.60      | 126.50   |
| 22  | BA    | 2607 | G    | N3-C4-N9   | 5.31  | 129.19      | 126.00   |
| 22  | BA    | 2572 | A    | O5'-P-OP2  | -5.31 | 100.92      | 105.70   |
| 22  | BA    | 1640 | A    | N9-C4-C5   | 5.30  | 107.92      | 105.80   |
| 22  | DA    | 2425 | A    | P-O3'-C3'  | 5.30  | 126.06      | 119.70   |
| 22  | BA    | 2565 | A    | N9-C4-C5   | -5.30 | 103.68      | 105.80   |
| 22  | BA    | 491  | G    | N3-C4-N9   | -5.30 | 122.82      | 126.00   |
| 22  | BA    | 2825 | G    | C8-N9-C4   | -5.30 | 104.28      | 106.40   |
| 22  | BA    | 1763 | G    | C4-N9-C1'  | -5.30 | 119.61      | 126.50   |
| 22  | BA    | 510  | C    | OP1-P-O3'  | 5.29  | 116.83      | 105.20   |

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| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 22  | BA    | 773  | U    | C5-C4-O4    | 5.28  | 129.07      | 125.90   |
| 22  | BA    | 752  | A    | N9-C1'-C2'  | 5.27  | 120.85      | 114.00   |
| 22  | BA    | 561  | G    | C4-C5-N7    | 5.26  | 112.91      | 110.80   |
| 22  | BA    | 561  | G    | C4-N9-C1'   | -5.26 | 119.66      | 126.50   |
| 22  | BA    | 1567 | G    | C4-C5-N7    | 5.26  | 112.90      | 110.80   |
| 22  | BA    | 1817 | G    | C8-N9-C4    | 5.26  | 108.50      | 106.40   |
| 1   | CA    | 47   | C    | C6-N1-C2    | 5.26  | 122.40      | 120.30   |
| 22  | BA    | 984  | A    | O4'-C1'-N9  | 5.25  | 112.40      | 108.20   |
| 22  | BA    | 2585 | U    | C5'-C4'-O4' | 5.25  | 115.40      | 109.10   |
| 22  | BA    | 942  | G    | N1-C6-O6    | 5.25  | 123.05      | 119.90   |
| 22  | DA    | 757  | G    | N3-C4-C5    | 5.25  | 131.22      | 128.60   |
| 22  | BA    | 1758 | U    | N3-C4-O4    | -5.25 | 115.73      | 119.40   |
| 22  | BA    | 2646 | C    | C6-N1-C2    | -5.25 | 118.20      | 120.30   |
| 22  | BA    | 2869 | G    | N1-C6-O6    | 5.24  | 123.04      | 119.90   |
| 22  | DA    | 2501 | C    | O4'-C1'-N1  | 5.23  | 112.39      | 108.20   |
| 37  | BP    | 103  | ARG  | NE-CZ-NH2   | -5.23 | 117.69      | 120.30   |
| 22  | BA    | 787  | C    | C6-N1-C2    | 5.22  | 122.39      | 120.30   |
| 22  | BA    | 1961 | C    | C6-N1-C2    | 5.22  | 122.39      | 120.30   |
| 22  | BA    | 806  | C    | C6-N1-C2    | -5.22 | 118.21      | 120.30   |
| 22  | BA    | 1997 | C    | C2-N3-C4    | -5.22 | 117.29      | 119.90   |
| 22  | BA    | 794  | A    | C5-C6-N6    | -5.21 | 119.53      | 123.70   |
| 22  | BA    | 2076 | U    | N1-C2-N3    | 5.21  | 118.03      | 114.90   |
| 22  | BA    | 2813 | A    | C8-N9-C4    | 5.21  | 107.89      | 105.80   |
| 22  | BA    | 1678 | A    | N1-C6-N6    | 5.21  | 121.73      | 118.60   |
| 22  | BA    | 2275 | C    | O5'-P-OP2   | -5.21 | 101.01      | 105.70   |
| 22  | BA    | 752  | A    | C4-N9-C1'   | 5.21  | 135.68      | 126.30   |
| 22  | DA    | 2447 | G    | O4'-C1'-N9  | 5.21  | 112.37      | 108.20   |
| 22  | BA    | 867  | C    | N1-C2-O2    | -5.21 | 115.78      | 118.90   |
| 22  | BA    | 919  | U    | C5-C4-O4    | -5.21 | 122.78      | 125.90   |
| 22  | BA    | 1007 | C    | O5'-P-OP1   | -5.21 | 101.02      | 105.70   |
| 22  | BA    | 2505 | G    | N9-C4-C5    | 5.21  | 107.48      | 105.40   |
| 22  | BA    | 1956 | U    | N1-C2-O2    | -5.20 | 119.16      | 122.80   |
| 22  | BA    | 481  | G    | O4'-C1'-N9  | 5.20  | 112.36      | 108.20   |
| 22  | BA    | 1653 | G    | C8-N9-C4    | -5.20 | 104.32      | 106.40   |
| 22  | BA    | 961  | C    | O5'-P-OP2   | -5.20 | 101.03      | 105.70   |
| 22  | BA    | 1681 | G    | N3-C2-N2    | -5.20 | 116.26      | 119.90   |
| 22  | BA    | 1377 | G    | N3-C4-C5    | -5.19 | 126.00      | 128.60   |
| 22  | BA    | 1389 | G    | C8-N9-C4    | 5.19  | 108.48      | 106.40   |
| 22  | BA    | 2636 | C    | C5-C4-N4    | -5.19 | 116.56      | 120.20   |
| 22  | BA    | 1262 | A    | OP1-P-O3'   | 5.19  | 116.62      | 105.20   |
| 22  | BA    | 2813 | A    | C2-N3-C4    | -5.19 | 108.00      | 110.60   |
| 22  | BA    | 1121 | C    | C2-N3-C4    | -5.18 | 117.31      | 119.90   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 22  | BA    | 537  | G    | N1-C6-O6   | 5.18  | 123.01      | 119.90   |
| 22  | BA    | 578  | G    | N1-C6-O6   | 5.18  | 123.01      | 119.90   |
| 22  | BA    | 740  | C    | OP1-P-OP2  | -5.17 | 111.85      | 119.60   |
| 22  | BA    | 914  | G    | N1-C6-O6   | 5.17  | 123.00      | 119.90   |
| 22  | BA    | 708  | G    | N1-C6-O6   | 5.16  | 123.00      | 119.90   |
| 22  | BA    | 2858 | C    | N3-C4-C5   | 5.16  | 123.97      | 121.90   |
| 22  | BA    | 41   | C    | C6-N1-C2   | 5.16  | 122.36      | 120.30   |
| 29  | BH    | 121  | VAL  | C-N-CA     | 5.16  | 134.59      | 121.70   |
| 22  | BA    | 1658 | C    | N1-C2-O2   | -5.16 | 115.81      | 118.90   |
| 1   | AA    | 1502 | A    | O5'-P-OP2  | -5.16 | 101.06      | 105.70   |
| 22  | BA    | 1936 | A    | C4-C5-N7   | 5.16  | 113.28      | 110.70   |
| 22  | BA    | 1784 | A    | C2-N3-C4   | -5.15 | 108.03      | 110.60   |
| 1   | AA    | 330  | C    | N3-C4-N4   | -5.15 | 114.40      | 118.00   |
| 22  | BA    | 1985 | C    | C5-C6-N1   | -5.15 | 118.43      | 121.00   |
| 1   | AA    | 1514 | G    | N1-C6-O6   | 5.15  | 122.99      | 119.90   |
| 22  | BA    | 1223 | G    | N3-C4-N9   | -5.15 | 122.91      | 126.00   |
| 22  | BA    | 2757 | A    | N1-C6-N6   | 5.14  | 121.69      | 118.60   |
| 22  | BA    | 1296 | G    | N1-C2-N2   | -5.14 | 111.57      | 116.20   |
| 22  | BA    | 708  | G    | C5-C6-O6   | -5.14 | 125.52      | 128.60   |
| 22  | BA    | 2063 | C    | N1-C2-O2   | 5.14  | 121.98      | 118.90   |
| 23  | BB    | 85   | G    | C8-N9-C4   | 5.14  | 108.45      | 106.40   |
| 22  | BA    | 492  | A    | C8-N9-C4   | 5.13  | 107.85      | 105.80   |
| 22  | BA    | 2036 | C    | N3-C4-C5   | 5.13  | 123.95      | 121.90   |
| 1   | AA    | 365  | U    | C5-C6-N1   | -5.12 | 120.14      | 122.70   |
| 22  | BA    | 2499 | C    | C5-C4-N4   | -5.12 | 116.61      | 120.20   |
| 22  | DA    | 1821 | A    | O5'-P-OP2  | -5.12 | 101.09      | 105.70   |
| 22  | BA    | 1215 | G    | C5-C6-O6   | 5.12  | 131.67      | 128.60   |
| 22  | BA    | 2020 | A    | N1-C6-N6   | -5.12 | 115.53      | 118.60   |
| 22  | BA    | 2283 | C    | C2-N1-C1'  | -5.11 | 113.18      | 118.80   |
| 22  | BA    | 2874 | C    | C2-N3-C4   | -5.11 | 117.34      | 119.90   |
| 22  | BA    | 2814 | A    | C5-C6-N6   | -5.11 | 119.61      | 123.70   |
| 22  | BA    | 1377 | G    | C8-N9-C4   | -5.11 | 104.36      | 106.40   |
| 22  | BA    | 528  | A    | O4'-C1'-N9 | -5.11 | 104.11      | 108.20   |
| 22  | BA    | 1401 | G    | N1-C6-O6   | 5.11  | 122.96      | 119.90   |
| 22  | BA    | 2276 | G    | N1-C6-O6   | -5.10 | 116.84      | 119.90   |
| 22  | BA    | 569  | U    | N1-C2-O2   | -5.10 | 119.23      | 122.80   |
| 22  | BA    | 1987 | A    | N1-C6-N6   | -5.10 | 115.54      | 118.60   |
| 22  | BA    | 1949 | G    | N3-C4-N9   | -5.10 | 122.94      | 126.00   |
| 22  | BA    | 1291 | C    | O5'-P-OP2  | -5.09 | 101.11      | 105.70   |
| 22  | BA    | 1311 | G    | C4-C5-N7   | 5.09  | 112.84      | 110.80   |
| 22  | BA    | 805  | G    | C8-N9-C4   | 5.09  | 108.44      | 106.40   |
| 22  | BA    | 2898 | U    | O5'-P-OP2  | -5.09 | 101.12      | 105.70   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 22  | BA    | 1357 | C    | N1-C2-O2   | -5.09 | 115.85      | 118.90   |
| 22  | BA    | 2272 | U    | C5-C4-O4   | -5.09 | 122.85      | 125.90   |
| 1   | AA    | 1279 | G    | N7-C8-N9   | 5.08  | 115.64      | 113.10   |
| 22  | BA    | 1669 | A    | C5-C6-N1   | 5.08  | 120.24      | 117.70   |
| 22  | BA    | 2721 | A    | C5-C6-N1   | 5.08  | 120.24      | 117.70   |
| 22  | BA    | 2633 | G    | C2-N3-C4   | -5.07 | 109.36      | 111.90   |
| 23  | BB    | 79   | G    | O5'-P-OP1  | 5.07  | 116.79      | 110.70   |
| 1   | AA    | 890  | G    | O4'-C1'-N9 | 5.07  | 112.26      | 108.20   |
| 22  | BA    | 811  | U    | N3-C4-O4   | -5.07 | 115.85      | 119.40   |
| 22  | BA    | 1616 | A    | C5-N7-C8   | -5.07 | 101.36      | 103.90   |
| 22  | BA    | 2278 | A    | C8-N9-C4   | 5.07  | 107.83      | 105.80   |
| 22  | BA    | 1787 | A    | C2-N3-C4   | -5.05 | 108.07      | 110.60   |
| 22  | BA    | 2089 | C    | N3-C4-C5   | 5.05  | 123.92      | 121.90   |
| 22  | DA    | 2245 | U    | C6-N1-C1'  | 5.04  | 128.26      | 121.20   |
| 22  | BA    | 2606 | C    | C2-N3-C4   | -5.04 | 117.38      | 119.90   |
| 22  | BA    | 1783 | A    | O5'-P-OP1  | 5.04  | 116.75      | 110.70   |
| 22  | BA    | 2066 | C    | OP1-P-O3'  | 5.04  | 116.28      | 105.20   |
| 22  | BA    | 2447 | G    | O4'-C1'-N9 | 5.04  | 112.23      | 108.20   |
| 22  | BA    | 1338 | G    | C8-N9-C4   | -5.04 | 104.39      | 106.40   |
| 22  | BA    | 1669 | A    | C2-N3-C4   | 5.04  | 113.12      | 110.60   |
| 22  | BA    | 1452 | G    | N3-C4-C5   | 5.03  | 131.12      | 128.60   |
| 22  | BA    | 1324 | G    | C5-C6-O6   | -5.03 | 125.58      | 128.60   |
| 22  | BA    | 2440 | C    | N3-C4-C5   | 5.03  | 123.91      | 121.90   |
| 22  | BA    | 2607 | G    | N1-C6-O6   | 5.03  | 122.92      | 119.90   |
| 22  | BA    | 767  | U    | O5'-P-OP2  | -5.02 | 101.18      | 105.70   |
| 22  | BA    | 2774 | C    | C5-C4-N4   | -5.02 | 116.69      | 120.20   |
| 1   | AA    | 1201 | A    | P-O3'-C3'  | 5.02  | 125.72      | 119.70   |
| 22  | BA    | 686  | U    | C2-N1-C1'  | -5.02 | 111.68      | 117.70   |
| 22  | BA    | 786  | C    | C6-N1-C2   | 5.02  | 122.31      | 120.30   |
| 22  | BA    | 2293 | G    | O5'-P-OP2  | -5.02 | 101.18      | 105.70   |
| 22  | BA    | 919  | U    | N3-C4-O4   | 5.02  | 122.91      | 119.40   |
| 22  | BA    | 1786 | A    | O5'-P-OP2  | -5.01 | 101.19      | 105.70   |
| 22  | BA    | 2592 | G    | C8-N9-C4   | -5.01 | 104.39      | 106.40   |
| 23  | BB    | 98   | G    | O5'-P-OP2  | -5.01 | 101.19      | 105.70   |
| 22  | BA    | 1282 | U    | N3-C2-O2   | 5.01  | 125.71      | 122.20   |
| 22  | BA    | 1677 | A    | C4-C5-N7   | 5.01  | 113.20      | 110.70   |
| 22  | BA    | 1774 | C    | N1-C2-O2   | -5.00 | 115.90      | 118.90   |
| 1   | CA    | 536  | C    | C6-N1-C2   | 5.00  | 122.30      | 120.30   |

There are no chirality outliers.

All (8) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 5   | AE    | 152 | MET  | Peptide |
| 11  | AK    | 126 | LYS  | Peptide |
| 25  | BD    | 151 | THR  | Peptide |
| 4   | CD    | 152 | GLN  | Peptide |
| 5   | CE    | 102 | GLY  | Peptide |
| 6   | CF    | 54  | LEU  | Peptide |
| 12  | CL    | 24  | LEU  | Peptide |
| 25  | DD    | 151 | 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    | 32995 | 0        | 16607    | 1101    | 3            |
| 1   | CA    | 33015 | 0        | 16617    | 1197    | 0            |
| 2   | AB    | 1705  | 0        | 1732     | 163     | 0            |
| 2   | CB    | 1705  | 0        | 1732     | 125     | 0            |
| 3   | AC    | 1625  | 0        | 1696     | 81      | 0            |
| 3   | CC    | 1625  | 0        | 1696     | 76      | 0            |
| 4   | AD    | 1643  | 0        | 1707     | 138     | 0            |
| 4   | CD    | 1643  | 0        | 1707     | 144     | 0            |
| 5   | AE    | 1106  | 0        | 1148     | 98      | 0            |
| 5   | CE    | 1106  | 0        | 1148     | 111     | 0            |
| 6   | AF    | 818   | 0        | 808      | 52      | 0            |
| 6   | CF    | 818   | 0        | 808      | 62      | 0            |
| 7   | AG    | 1182  | 0        | 1238     | 56      | 0            |
| 7   | CG    | 1182  | 0        | 1238     | 70      | 0            |
| 8   | AH    | 979   | 0        | 1031     | 74      | 0            |
| 8   | CH    | 979   | 0        | 1031     | 49      | 0            |
| 9   | AI    | 1022  | 0        | 1070     | 96      | 0            |
| 9   | CI    | 1022  | 0        | 1070     | 76      | 0            |
| 10  | AJ    | 787   | 0        | 828      | 97      | 0            |
| 10  | CJ    | 787   | 0        | 828      | 49      | 0            |
| 11  | AK    | 877   | 0        | 887      | 70      | 0            |
| 11  | CK    | 877   | 0        | 887      | 62      | 0            |
| 12  | AL    | 955   | 0        | 1016     | 57      | 0            |
| 12  | CL    | 955   | 0        | 1016     | 70      | 0            |
| 13  | AM    | 884   | 0        | 941      | 63      | 0            |
| 13  | CM    | 884   | 0        | 941      | 56      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 14  | AN    | 774   | 0        | 824      | 72      | 0            |
| 14  | CN    | 774   | 0        | 824      | 53      | 0            |
| 15  | AO    | 710   | 0        | 728      | 38      | 0            |
| 15  | CO    | 710   | 0        | 728      | 31      | 0            |
| 16  | AP    | 649   | 0        | 666      | 61      | 0            |
| 16  | CP    | 649   | 0        | 666      | 33      | 0            |
| 17  | AQ    | 649   | 0        | 691      | 71      | 0            |
| 17  | CQ    | 649   | 0        | 691      | 50      | 0            |
| 18  | AR    | 456   | 0        | 478      | 19      | 0            |
| 18  | CR    | 456   | 0        | 478      | 23      | 0            |
| 19  | AS    | 638   | 0        | 665      | 50      | 0            |
| 19  | CS    | 638   | 0        | 665      | 37      | 0            |
| 20  | AT    | 665   | 0        | 714      | 60      | 0            |
| 20  | CT    | 665   | 0        | 714      | 49      | 0            |
| 21  | AU    | 426   | 0        | 449      | 51      | 0            |
| 21  | CU    | 426   | 0        | 449      | 50      | 0            |
| 22  | BA    | 62195 | 0        | 31280    | 1688    | 0            |
| 22  | DA    | 62195 | 0        | 31280    | 2474    | 0            |
| 23  | BB    | 2549  | 0        | 1291     | 64      | 0            |
| 23  | DB    | 2529  | 0        | 1281     | 68      | 0            |
| 24  | BC    | 2083  | 0        | 2154     | 110     | 0            |
| 24  | DC    | 2083  | 0        | 2154     | 136     | 0            |
| 25  | BD    | 1565  | 0        | 1616     | 73      | 0            |
| 25  | DD    | 1565  | 0        | 1616     | 95      | 0            |
| 26  | BE    | 1552  | 0        | 1619     | 73      | 0            |
| 26  | DE    | 1552  | 0        | 1619     | 105     | 0            |
| 27  | BF    | 1411  | 0        | 1444     | 106     | 0            |
| 27  | DF    | 1411  | 0        | 1444     | 58      | 0            |
| 28  | BG    | 1323  | 0        | 1371     | 43      | 0            |
| 28  | DG    | 1323  | 0        | 1371     | 55      | 0            |
| 29  | BH    | 1110  | 0        | 1147     | 145     | 0            |
| 29  | DH    | 1110  | 0        | 1148     | 89      | 3            |
| 30  | BI    | 1032  | 0        | 1085     | 75      | 0            |
| 30  | DI    | 1032  | 0        | 1085     | 85      | 0            |
| 31  | BJ    | 1129  | 0        | 1162     | 44      | 0            |
| 31  | DJ    | 1129  | 0        | 1162     | 54      | 0            |
| 32  | BK    | 939   | 0        | 1012     | 43      | 0            |
| 32  | DK    | 939   | 0        | 1012     | 45      | 0            |
| 33  | BL    | 1045  | 0        | 1117     | 65      | 0            |
| 33  | DL    | 1045  | 0        | 1117     | 79      | 0            |
| 34  | BM    | 1074  | 0        | 1157     | 38      | 0            |
| 34  | DM    | 1074  | 0        | 1157     | 39      | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 35  | BN    | 961   | 0        | 1000     | 55      | 0            |
| 35  | DN    | 961   | 0        | 1000     | 77      | 0            |
| 36  | BO    | 892   | 0        | 923      | 51      | 0            |
| 36  | DO    | 892   | 0        | 923      | 44      | 0            |
| 37  | BP    | 917   | 0        | 962      | 42      | 0            |
| 37  | DP    | 917   | 0        | 962      | 60      | 0            |
| 38  | BQ    | 947   | 0        | 1019     | 50      | 0            |
| 38  | DQ    | 947   | 0        | 1019     | 50      | 0            |
| 39  | BR    | 816   | 0        | 839      | 68      | 0            |
| 39  | DR    | 816   | 0        | 839      | 42      | 0            |
| 40  | BS    | 857   | 0        | 922      | 43      | 0            |
| 40  | DS    | 857   | 0        | 922      | 42      | 0            |
| 41  | BT    | 739   | 0        | 807      | 52      | 0            |
| 41  | DT    | 739   | 0        | 807      | 60      | 0            |
| 42  | BU    | 780   | 0        | 831      | 40      | 0            |
| 42  | DU    | 780   | 0        | 831      | 69      | 0            |
| 43  | BV    | 753   | 0        | 780      | 33      | 0            |
| 43  | DV    | 753   | 0        | 780      | 24      | 0            |
| 44  | BW    | 580   | 0        | 594      | 15      | 0            |
| 44  | DW    | 569   | 0        | 581      | 24      | 0            |
| 45  | BX    | 625   | 0        | 652      | 19      | 0            |
| 45  | DX    | 625   | 0        | 652      | 44      | 0            |
| 46  | BY    | 509   | 0        | 543      | 34      | 0            |
| 46  | DY    | 509   | 0        | 543      | 29      | 0            |
| 47  | BZ    | 449   | 0        | 488      | 13      | 0            |
| 47  | DZ    | 449   | 0        | 488      | 22      | 0            |
| 48  | B0    | 444   | 0        | 458      | 24      | 0            |
| 48  | D0    | 444   | 0        | 458      | 26      | 0            |
| 49  | B1    | 410   | 0        | 440      | 30      | 0            |
| 49  | D1    | 410   | 0        | 440      | 21      | 0            |
| 50  | B2    | 377   | 0        | 418      | 13      | 0            |
| 50  | D2    | 377   | 0        | 418      | 33      | 0            |
| 51  | B3    | 504   | 0        | 572      | 25      | 0            |
| 51  | D3    | 504   | 0        | 572      | 24      | 0            |
| 52  | B4    | 302   | 0        | 340      | 12      | 0            |
| 52  | D4    | 302   | 0        | 340      | 15      | 0            |
| 53  | B5    | 1142  | 0        | 865      | 66      | 0            |
| 54  | AA    | 70    | 0        | 0        | 0       | 0            |
| 54  | AM    | 1     | 0        | 0        | 0       | 0            |
| 54  | AN    | 1     | 0        | 0        | 0       | 0            |
| 54  | BA    | 194   | 0        | 0        | 0       | 0            |
| 54  | BB    | 4     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 54  | BQ    | 1     | 0        | 0        | 0       | 0            |
| 54  | CA    | 56    | 0        | 0        | 0       | 0            |
| 54  | D2    | 1     | 0        | 0        | 0       | 0            |
| 54  | DA    | 164   | 0        | 0        | 0       | 0            |
| 54  | DB    | 3     | 0        | 0        | 0       | 0            |
| 54  | DL    | 1     | 0        | 0        | 0       | 0            |
| 54  | DQ    | 1     | 0        | 0        | 0       | 0            |
| 55  | BA    | 48    | 0        | 50       | 11      | 0            |
| 55  | DA    | 48    | 0        | 50       | 27      | 0            |
| 56  | B4    | 1     | 0        | 0        | 0       | 0            |
| 56  | D4    | 1     | 0        | 0        | 0       | 0            |
| 57  | AA    | 195   | 0        | 0        | 19      | 0            |
| 57  | AE    | 1     | 0        | 0        | 0       | 0            |
| 57  | AL    | 1     | 0        | 0        | 0       | 0            |
| 57  | AN    | 3     | 0        | 0        | 0       | 0            |
| 57  | AT    | 2     | 0        | 0        | 0       | 0            |
| 57  | AU    | 1     | 0        | 0        | 0       | 0            |
| 57  | B2    | 1     | 0        | 0        | 0       | 0            |
| 57  | B3    | 3     | 0        | 0        | 0       | 0            |
| 57  | B4    | 2     | 0        | 0        | 0       | 0            |
| 57  | BA    | 615   | 0        | 0        | 86      | 0            |
| 57  | BB    | 13    | 0        | 0        | 1       | 0            |
| 57  | BC    | 8     | 0        | 0        | 4       | 0            |
| 57  | BD    | 3     | 0        | 0        | 2       | 0            |
| 57  | BE    | 2     | 0        | 0        | 0       | 0            |
| 57  | BF    | 1     | 0        | 0        | 1       | 0            |
| 57  | BL    | 7     | 0        | 0        | 0       | 0            |
| 57  | BN    | 5     | 0        | 0        | 0       | 0            |
| 57  | BQ    | 1     | 0        | 0        | 0       | 0            |
| 57  | BS    | 1     | 0        | 0        | 0       | 0            |
| 57  | BT    | 1     | 0        | 0        | 0       | 0            |
| 57  | BU    | 1     | 0        | 0        | 0       | 0            |
| 57  | BV    | 1     | 0        | 0        | 0       | 0            |
| 57  | CA    | 193   | 0        | 0        | 17      | 0            |
| 57  | CL    | 1     | 0        | 0        | 0       | 0            |
| 57  | CN    | 1     | 0        | 0        | 0       | 0            |
| 57  | CT    | 2     | 0        | 0        | 0       | 0            |
| 57  | CU    | 1     | 0        | 0        | 1       | 0            |
| 57  | D2    | 1     | 0        | 0        | 1       | 0            |
| 57  | D3    | 1     | 0        | 0        | 0       | 0            |
| 57  | D4    | 1     | 0        | 0        | 1       | 0            |
| 57  | DA    | 608   | 0        | 0        | 96      | 0            |

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| Mol | Chain | Non-H  | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 57  | DB    | 13     | 0        | 0        | 4       | 0            |
| 57  | DC    | 10     | 0        | 0        | 1       | 0            |
| 57  | DD    | 4      | 0        | 0        | 2       | 0            |
| 57  | DE    | 4      | 0        | 0        | 0       | 0            |
| 57  | DJ    | 1      | 0        | 0        | 0       | 0            |
| 57  | DL    | 4      | 0        | 0        | 1       | 0            |
| 57  | DN    | 2      | 0        | 0        | 0       | 0            |
| 57  | DS    | 2      | 0        | 0        | 0       | 0            |
| 57  | DT    | 3      | 0        | 0        | 1       | 0            |
| 57  | DU    | 1      | 0        | 0        | 0       | 0            |
| 57  | DV    | 1      | 0        | 0        | 0       | 0            |
| All | All   | 288276 | 0        | 192887   | 11371   | 3            |

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 24.

All (11371) 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) |
|---------------------|---------------------|--------------------------|-------------------|
| 29:BH:117:LEU:O     | 29:BH:121:VAL:HG23  | 1.34                     | 1.22              |
| 22:DA:2711:A:OP2    | 57:DA:3546:HOH:O    | 1.61                     | 1.18              |
| 1:AA:111:G:O6       | 1:AA:330:C:N4       | 1.78                     | 1.16              |
| 22:BA:627:A:OP1     | 33:BL:78:ARG:NH1    | 1.79                     | 1.16              |
| 22:BA:730:A:OP2     | 57:BA:3695:HOH:O    | 1.61                     | 1.16              |
| 25:DD:151:THR:O     | 25:DD:153:GLY:N     | 1.79                     | 1.14              |
| 29:BH:117:LEU:O     | 29:BH:121:VAL:CG2   | 1.95                     | 1.14              |
| 22:BA:1153:C:OP2    | 57:BA:3361:HOH:O    | 1.66                     | 1.12              |
| 22:BA:1603:A:OP1    | 57:BA:3414:HOH:O    | 1.64                     | 1.11              |
| 22:BA:2498:C:OP2    | 57:BA:3686:HOH:O    | 1.68                     | 1.09              |
| 22:BA:1395:A:OP1    | 57:BA:3414:HOH:O    | 1.71                     | 1.09              |
| 29:BH:123:ARG:O     | 29:BH:124:THR:CG2   | 2.01                     | 1.09              |
| 5:CE:101:GLU:O      | 5:CE:103:THR:N      | 1.86                     | 1.08              |
| 22:BA:1342:A:OP2    | 57:BA:3714:HOH:O    | 1.71                     | 1.06              |
| 22:BA:2720:U:OP1    | 37:BP:53:ARG:NH2    | 1.89                     | 1.06              |
| 22:BA:842:U:O4      | 57:BA:3588:HOH:O    | 1.73                     | 1.04              |
| 1:AA:533:A:OP1      | 57:AA:1849:HOH:O    | 1.76                     | 1.04              |
| 22:BA:1602:U:O4     | 57:BA:3714:HOH:O    | 1.76                     | 1.04              |
| 22:DA:621:A:OP2     | 57:DA:3292:HOH:O    | 1.74                     | 1.03              |
| 55:DA:3001:DOL:H463 | 55:DA:3001:DOL:H483 | 1.06                     | 1.03              |
| 22:BA:731:C:OP2     | 57:BA:3695:HOH:O    | 1.76                     | 1.03              |
| 22:DA:789:A:N1      | 57:DA:3310:HOH:O    | 1.89                     | 1.03              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 22:BA:1062:G:N2    | 22:BA:1077:A:N1     | 2.07                     | 1.02              |
| 22:DA:602:A:O2'    | 22:DA:604:G:O2'     | 1.77                     | 1.01              |
| 1:AA:800:G:O6      | 57:AA:1814:HOH:O    | 1.79                     | 1.01              |
| 36:BO:31:THR:O     | 36:BO:102:ARG:NH1   | 1.93                     | 1.01              |
| 22:DA:2056:G:OP2   | 57:DA:3485:HOH:O    | 1.77                     | 1.00              |
| 55:DA:3001:DOL:HC1 | 55:DA:3001:DOL:H431 | 1.42                     | 1.00              |
| 29:BH:117:LEU:HD21 | 29:BH:121:VAL:H     | 1.23                     | 1.00              |
| 22:DA:842:U:O4     | 57:DA:3577:HOH:O    | 1.77                     | 1.00              |
| 1:AA:516:U:O4      | 57:AA:1849:HOH:O    | 1.78                     | 0.99              |
| 22:DA:2349:G:OP1   | 51:D3:45:ARG:NH2    | 1.95                     | 0.99              |
| 23:DB:28:C:OP1     | 36:DO:36:TYR:OH     | 1.79                     | 0.99              |
| 29:BH:123:ARG:O    | 29:BH:124:THR:HG23  | 1.61                     | 0.99              |
| 55:DA:3001:DOL:C48 | 55:DA:3001:DOL:H463 | 1.91                     | 0.99              |
| 22:DA:2504:U:C5    | 55:DA:3001:DOL:H161 | 1.98                     | 0.98              |
| 22:BA:1509:A:O2'   | 22:BA:1510:G:OP2    | 1.81                     | 0.98              |
| 55:DA:3001:DOL:C46 | 55:DA:3001:DOL:H483 | 1.92                     | 0.98              |
| 5:CE:157:ARG:O     | 5:CE:159:LYS:N      | 1.96                     | 0.98              |
| 2:CB:73:LYS:O      | 2:CB:75:ALA:N       | 1.95                     | 0.98              |
| 22:BA:2428:G:OP1   | 57:BA:3701:HOH:O    | 1.80                     | 0.97              |
| 13:AM:11:ASP:OD1   | 13:AM:12:HIS:N      | 1.96                     | 0.97              |
| 4:CD:41:HIS:O      | 4:CD:43:ALA:N       | 1.98                     | 0.97              |
| 29:DH:40:THR:O     | 29:DH:42:LYS:N      | 1.98                     | 0.97              |
| 1:CA:858:G:N7      | 57:CA:1819:HOH:O    | 1.97                     | 0.96              |
| 1:CA:912:C:OP1     | 12:CL:43:LYS:NZ     | 1.97                     | 0.96              |
| 22:BA:2611:C:OP2   | 57:BA:3546:HOH:O    | 1.82                     | 0.96              |
| 22:BA:2269:G:OP1   | 57:BA:3515:HOH:O    | 1.84                     | 0.95              |
| 22:DA:1464:G:N7    | 57:DA:3633:HOH:O    | 1.99                     | 0.95              |
| 22:DA:450:G:O6     | 57:DA:3242:HOH:O    | 1.83                     | 0.95              |
| 2:AB:21:ARG:O      | 2:AB:23:TRP:N       | 1.99                     | 0.95              |
| 29:BH:120:GLY:C    | 29:BH:122:LEU:HA    | 1.85                     | 0.95              |
| 22:DA:1268:A:OP1   | 57:DA:3378:HOH:O    | 1.84                     | 0.95              |
| 22:DA:784:G:OP1    | 57:DA:3314:HOH:O    | 1.81                     | 0.95              |
| 22:DA:1378:A:O2'   | 22:DA:1380:G:N7     | 1.98                     | 0.95              |
| 4:CD:29:ASP:O      | 4:CD:31:LYS:N       | 1.99                     | 0.95              |
| 22:DA:1010:A:OP2   | 57:DA:3778:HOH:O    | 1.85                     | 0.94              |
| 2:AB:193:PRO:O     | 2:AB:195:GLY:N      | 2.01                     | 0.94              |
| 22:BA:1923:U:H2'   | 22:BA:1924:C:H5'    | 1.47                     | 0.94              |
| 22:DA:514:A:N3     | 22:DA:581:C:O2'     | 2.00                     | 0.94              |
| 22:DA:2243:U:OP1   | 57:DA:3737:HOH:O    | 1.85                     | 0.93              |
| 22:DA:299:A:N3     | 22:DA:319:G:O2'     | 2.00                     | 0.93              |
| 22:BA:1093:G:N3    | 22:BA:1098:A:N6     | 2.16                     | 0.93              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:DA:729:G:OP2    | 24:DC:207:LYS:NZ   | 2.02                     | 0.93              |
| 48:B0:20:ASP:N     | 48:B0:20:ASP:OD2   | 2.00                     | 0.93              |
| 22:DA:1378:A:O2'   | 57:DA:3751:HOH:O   | 1.86                     | 0.93              |
| 22:DA:1050:A:N6    | 22:DA:1109:C:O2    | 2.01                     | 0.93              |
| 22:BA:1909:C:N4    | 22:BA:1921:G:O6    | 2.02                     | 0.93              |
| 29:BH:27:ARG:NH2   | 45:BX:60:ASP:OD2   | 2.02                     | 0.92              |
| 6:AF:91:ARG:O      | 6:AF:92:THR:OG1    | 1.86                     | 0.92              |
| 1:AA:537:G:OP1     | 12:AL:110:ARG:NH2  | 2.02                     | 0.92              |
| 40:DS:28:LYS:O     | 40:DS:30:SER:N     | 2.02                     | 0.92              |
| 22:BA:819:A:OP2    | 22:BA:1187:G:N2    | 2.02                     | 0.91              |
| 1:CA:1500:A:OP2    | 57:CA:1884:HOH:O   | 1.87                     | 0.91              |
| 1:CA:1198:G:N7     | 57:CA:1853:HOH:O   | 2.02                     | 0.91              |
| 22:BA:517:C:OP2    | 48:B0:10:ARG:NH2   | 2.03                     | 0.91              |
| 22:DA:370:G:OP2    | 57:DA:3556:HOH:O   | 1.88                     | 0.91              |
| 22:BA:1998:A:OP2   | 25:BD:141:ARG:NH2  | 2.04                     | 0.91              |
| 22:DA:528:A:OP1    | 57:DA:3246:HOH:O   | 1.89                     | 0.91              |
| 1:AA:880:C:OP1     | 12:AL:9:ARG:NH1    | 2.04                     | 0.90              |
| 29:DH:83:LYS:HG3   | 29:DH:149:GLU:CG   | 2.02                     | 0.90              |
| 1:AA:1198:G:N7     | 57:AA:1788:HOH:O   | 2.03                     | 0.90              |
| 1:AA:1232:U:OP1    | 9:AI:126:GLN:NE2   | 2.04                     | 0.90              |
| 4:CD:174:ASP:OD1   | 4:CD:175:ALA:N     | 2.04                     | 0.90              |
| 22:BA:2728:U:O2'   | 22:BA:2729:G:OP2   | 1.90                     | 0.90              |
| 22:DA:1995:U:OP1   | 57:DA:3805:HOH:O   | 1.89                     | 0.90              |
| 7:AG:55:GLY:O      | 7:AG:57:SER:N      | 2.05                     | 0.90              |
| 3:AC:36:ASP:OD1    | 3:AC:59:ARG:NH1    | 2.04                     | 0.90              |
| 22:DA:2714:G:OP2   | 57:DA:3546:HOH:O   | 1.87                     | 0.90              |
| 22:BA:1924:C:H2'   | 22:BA:1925:C:H5"   | 1.55                     | 0.89              |
| 22:BA:2445:G:OP1   | 26:BE:69:ARG:NH2   | 2.05                     | 0.89              |
| 41:DT:21:SER:O     | 41:DT:23:ALA:N     | 2.04                     | 0.89              |
| 22:DA:188:G:O2'    | 22:DA:1365:A:N6    | 2.06                     | 0.89              |
| 40:BS:53:SER:O     | 40:BS:57:ASN:ND2   | 2.06                     | 0.89              |
| 28:DG:158:LYS:O    | 28:DG:160:LYS:N    | 2.06                     | 0.89              |
| 5:AE:157:ARG:O     | 5:AE:159:LYS:N     | 2.04                     | 0.89              |
| 55:DA:3001:DOL:HC1 | 55:DA:3001:DOL:C43 | 2.00                     | 0.89              |
| 22:DA:2615:U:OP1   | 57:DA:3745:HOH:O   | 1.89                     | 0.89              |
| 22:DA:300:A:N6     | 57:DA:3551:HOH:O   | 2.06                     | 0.89              |
| 25:BD:140:HIS:NE2  | 57:BD:302:HOH:O    | 2.06                     | 0.88              |
| 1:CA:32:A:C2       | 1:CA:33:A:C5       | 2.60                     | 0.88              |
| 22:DA:18:U:O4      | 57:DA:3205:HOH:O   | 1.92                     | 0.88              |
| 1:AA:1312:G:N7     | 19:AS:3:ARG:N      | 2.21                     | 0.88              |
| 22:BA:944:C:OP2    | 57:BA:3261:HOH:O   | 1.90                     | 0.88              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:DA:2271:G:O6    | 57:DA:3508:HOH:O   | 1.89                     | 0.88              |
| 22:DA:2627:G:O2'   | 22:DA:2781:A:N1    | 2.06                     | 0.88              |
| 29:BH:123:ARG:O    | 29:BH:124:THR:HG22 | 1.74                     | 0.88              |
| 39:DR:101:ILE:O    | 39:DR:103:ALA:N    | 2.06                     | 0.88              |
| 29:BH:117:LEU:C    | 29:BH:121:VAL:HG23 | 1.93                     | 0.87              |
| 24:BC:70:ASN:O     | 24:BC:72:ASP:N     | 2.07                     | 0.87              |
| 23:DB:43:C:O2      | 27:DF:92:ARG:NH2   | 2.07                     | 0.87              |
| 20:CT:5:LYS:O      | 20:CT:7:ALA:N      | 2.07                     | 0.87              |
| 22:DA:1613:G:O6    | 57:DA:3638:HOH:O   | 1.90                     | 0.87              |
| 22:DA:2588:G:OP1   | 57:DA:3314:HOH:O   | 1.92                     | 0.87              |
| 31:DJ:80:HIS:O     | 31:DJ:82:GLY:N     | 2.07                     | 0.87              |
| 1:AA:928:G:O2'     | 1:AA:1533:C:OP1    | 1.93                     | 0.87              |
| 22:DA:1300:G:O6    | 22:DA:1626:A:O2'   | 1.91                     | 0.87              |
| 29:BH:123:ARG:HD3  | 1:CA:358:U:OP1     | 1.74                     | 0.87              |
| 17:CQ:19:LYS:O     | 17:CQ:71:LYS:NZ    | 2.08                     | 0.87              |
| 29:DH:83:LYS:HG3   | 29:DH:149:GLU:HG2  | 1.56                     | 0.86              |
| 22:BA:1073:A:H3'   | 22:BA:1074:G:C5'   | 2.05                     | 0.86              |
| 22:DA:182:A:HO2'   | 22:DA:433:C:HO2'   | 1.11                     | 0.86              |
| 1:AA:452:A:N6      | 1:AA:480:U:O2      | 2.08                     | 0.86              |
| 1:AA:825:A:O2'     | 8:AH:13:ARG:NH1    | 2.07                     | 0.86              |
| 22:BA:1001:A:OP2   | 57:BA:3736:HOH:O   | 1.93                     | 0.86              |
| 22:DA:182:A:O2'    | 22:DA:433:C:O2'    | 1.91                     | 0.86              |
| 1:AA:965:U:OP2     | 57:AA:1833:HOH:O   | 1.92                     | 0.86              |
| 1:CA:484:G:H4'     | 1:CA:485:U:O5'     | 1.75                     | 0.86              |
| 22:DA:613:A:O2'    | 22:DA:614:A:OP1    | 1.91                     | 0.86              |
| 1:AA:980:C:OP2     | 57:AA:1837:HOH:O   | 1.92                     | 0.86              |
| 3:AC:85:GLU:OE1    | 3:AC:88:ARG:NH1    | 2.07                     | 0.86              |
| 22:DA:310:A:O2'    | 22:DA:311:A:OP2    | 1.92                     | 0.86              |
| 9:CI:107:ASP:OD1   | 9:CI:109:ARG:NH1   | 2.09                     | 0.86              |
| 22:DA:1359:A:OP1   | 57:DA:3610:HOH:O   | 1.92                     | 0.86              |
| 22:BA:2116:G:O6    | 22:BA:2171:A:N6    | 2.09                     | 0.86              |
| 29:BH:147:VAL:HG12 | 29:BH:149:GLU:HG3  | 1.57                     | 0.86              |
| 22:DA:370:G:N7     | 57:DA:3555:HOH:O   | 2.08                     | 0.86              |
| 22:BA:1916:A:C4    | 22:BA:1917:U:H1'   | 2.11                     | 0.86              |
| 31:DJ:41:LYS:O     | 31:DJ:43:GLU:N     | 2.08                     | 0.86              |
| 1:CA:1256:A:O2'    | 1:CA:1278:G:O6     | 1.94                     | 0.85              |
| 22:DA:1287:A:O4'   | 35:DN:103:ARG:NH1  | 2.10                     | 0.85              |
| 22:BA:1064:C:N4    | 22:BA:1070:A:OP2   | 2.10                     | 0.85              |
| 4:CD:28:ILE:O      | 4:CD:31:LYS:NZ     | 2.08                     | 0.85              |
| 22:DA:258:G:O2'    | 33:DL:104:GLN:OE1  | 1.93                     | 0.85              |
| 47:DZ:52:SER:O     | 47:DZ:54:MET:N     | 2.08                     | 0.85              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 22:DA:2834:G:O6    | 22:DA:2879:A:O2'    | 1.95                     | 0.85              |
| 5:CE:102:GLY:O     | 5:CE:104:GLY:N      | 2.10                     | 0.85              |
| 22:DA:1439:A:OP2   | 57:DA:3627:HOH:O    | 1.94                     | 0.85              |
| 26:BE:7:ASP:OD2    | 26:BE:8:ALA:N       | 2.10                     | 0.85              |
| 28:DG:126:PRO:O    | 28:DG:127:THR:OG1   | 1.92                     | 0.85              |
| 14:CN:41:ARG:NH1   | 14:CN:42:TRP:O      | 2.10                     | 0.84              |
| 22:BA:1823:G:N7    | 57:BA:3659:HOH:O    | 2.10                     | 0.84              |
| 22:DA:83:A:OP2     | 42:DU:92:LYS:NZ     | 2.10                     | 0.84              |
| 17:AQ:17:MET:N     | 17:AQ:17:MET:SD     | 2.51                     | 0.84              |
| 23:DB:22:U:O4      | 57:DB:302:HOH:O     | 1.94                     | 0.84              |
| 18:CR:20:GLU:O     | 18:CR:22:ASP:N      | 2.10                     | 0.84              |
| 22:DA:1508:A:O2'   | 22:DA:1509:A:O4'    | 1.95                     | 0.84              |
| 34:DM:66:ARG:NH1   | 34:DM:104:GLU:OE1   | 2.11                     | 0.84              |
| 29:BH:117:LEU:HD21 | 29:BH:121:VAL:N     | 1.93                     | 0.84              |
| 29:BH:117:LEU:O    | 29:BH:119:ASN:N     | 2.07                     | 0.84              |
| 10:CJ:63:ASP:OD1   | 14:CN:85:ARG:NH1    | 2.10                     | 0.84              |
| 29:DH:82:SER:O     | 29:DH:84:ALA:N      | 2.10                     | 0.84              |
| 22:BA:1779:U:H5    | 22:BA:1784:A:N7     | 1.76                     | 0.84              |
| 22:BA:560:C:OP2    | 57:BA:3250:HOH:O    | 1.93                     | 0.84              |
| 35:DN:87:PHE:O     | 35:DN:89:SER:N      | 2.11                     | 0.84              |
| 22:DA:2505:G:OP2   | 55:DA:3001:DOL:HC17 | 1.77                     | 0.84              |
| 14:AN:33:ASP:O     | 14:AN:35:ASN:N      | 2.10                     | 0.84              |
| 4:AD:27:ALA:O      | 4:AD:31:LYS:NZ      | 2.10                     | 0.83              |
| 22:BA:797:G:O6     | 57:BA:3324:HOH:O    | 1.95                     | 0.83              |
| 22:DA:1344:U:O2'   | 22:DA:1345:C:OP2    | 1.96                     | 0.83              |
| 22:DA:990:A:N1     | 39:DR:78:ARG:NH1    | 2.26                     | 0.83              |
| 29:DH:94:ILE:HB    | 29:DH:122:LEU:HD12  | 1.60                     | 0.83              |
| 22:DA:58:G:OP1     | 41:DT:78:SER:OG     | 1.95                     | 0.83              |
| 1:CA:736:C:OP1     | 18:CR:61:ARG:NH1    | 2.10                     | 0.83              |
| 1:CA:319:G:O6      | 57:CA:1735:HOH:O    | 1.95                     | 0.83              |
| 22:DA:1667:G:O2'   | 22:DA:1991:U:O4     | 1.97                     | 0.83              |
| 22:BA:1179:G:N7    | 22:BA:1180:U:C6     | 2.47                     | 0.83              |
| 1:CA:201:G:N2      | 1:CA:469:C:O2       | 2.11                     | 0.83              |
| 9:AI:57:MET:N      | 9:AI:57:MET:SD      | 2.52                     | 0.83              |
| 22:BA:2757:A:N1    | 28:BG:67:THR:HG21   | 1.93                     | 0.82              |
| 20:CT:59:ASP:OD2   | 20:CT:76:LYS:NZ     | 2.11                     | 0.82              |
| 22:DA:581:C:OP2    | 38:DQ:33:ARG:NH1    | 2.12                     | 0.82              |
| 7:CG:93:PRO:O      | 7:CG:97:ASN:ND2     | 2.11                     | 0.82              |
| 50:D2:11:LYS:NZ    | 57:D2:201:HOH:O     | 2.10                     | 0.82              |
| 22:DA:1371:G:N7    | 57:DA:3399:HOH:O    | 2.11                     | 0.82              |
| 9:AI:42:GLU:O      | 9:AI:45:ARG:NH1     | 2.13                     | 0.82              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 29:BH:120:GLY:C     | 29:BH:122:LEU:CA    | 2.47                     | 0.82              |
| 26:DE:111:GLU:OE2   | 26:DE:114:ARG:NH1   | 2.13                     | 0.82              |
| 22:BA:2572:A:N7     | 25:BD:150:GLN:HG3   | 1.95                     | 0.82              |
| 1:CA:1046:A:N6      | 1:CA:1211:U:O2      | 2.13                     | 0.82              |
| 1:CA:495:A:C2       | 1:CA:496:A:C6       | 2.68                     | 0.82              |
| 1:CA:992:U:O4'      | 1:CA:993:G:N2       | 2.13                     | 0.82              |
| 1:CA:409:U:OP1      | 4:CD:24:GLY:HA3     | 1.78                     | 0.81              |
| 43:BV:80:HIS:CE1    | 43:BV:83:LYS:HG3    | 2.15                     | 0.81              |
| 1:CA:209:U:H4'      | 1:CA:210:C:OP2      | 1.80                     | 0.81              |
| 39:DR:8:GLY:O       | 39:DR:10:LYS:NZ     | 2.11                     | 0.81              |
| 22:BA:1603:A:OP1    | 57:BA:3412:HOH:O    | 1.97                     | 0.81              |
| 1:CA:1007:U:O4      | 1:CA:1022:A:N6      | 2.14                     | 0.81              |
| 22:DA:1269:A:OP2    | 57:DA:3385:HOH:O    | 1.98                     | 0.81              |
| 27:BF:40:VAL:O      | 27:BF:42:GLU:N      | 2.13                     | 0.81              |
| 23:DB:40:U:N3       | 23:DB:44:G:OP2      | 2.13                     | 0.81              |
| 41:BT:64:LYS:HA     | 41:BT:79:ASP:OD1    | 1.81                     | 0.81              |
| 22:DA:1817:G:OP1    | 24:DC:62:TYR:OH     | 1.99                     | 0.81              |
| 22:BA:974:G:H8      | 22:BA:990:A:H62     | 1.26                     | 0.81              |
| 22:DA:443:A:N7      | 26:DE:40:ARG:HG3    | 1.96                     | 0.81              |
| 1:CA:243:A:H4'      | 1:CA:244:U:C5'      | 2.10                     | 0.81              |
| 1:CA:243:A:H4'      | 1:CA:244:U:H5'      | 1.62                     | 0.81              |
| 22:BA:198:C:OP2     | 57:BA:3760:HOH:O    | 1.99                     | 0.80              |
| 1:CA:1308:U:OP1     | 13:CM:97:VAL:N      | 2.14                     | 0.80              |
| 22:DA:279:A:N6      | 22:DA:361:G:O2'     | 2.14                     | 0.80              |
| 22:DA:618:G:O6      | 57:DA:3291:HOH:O    | 2.00                     | 0.80              |
| 1:CA:205:A:N6       | 1:CA:213:G:O6       | 2.14                     | 0.80              |
| 1:AA:207:C:O2       | 1:AA:213:G:N2       | 2.14                     | 0.80              |
| 7:AG:80:VAL:O       | 7:AG:82:GLY:N       | 2.14                     | 0.80              |
| 22:BA:1061:U:O2'    | 22:BA:1062:G:O5'    | 1.98                     | 0.80              |
| 25:BD:77:ARG:NH2    | 25:BD:200:ASP:OD1   | 2.14                     | 0.80              |
| 1:CA:266:G:H3'      | 17:CQ:69:LYS:HB2    | 1.64                     | 0.80              |
| 5:CE:99:ALA:O       | 5:CE:101:GLU:N      | 2.14                     | 0.80              |
| 6:CF:91:ARG:O       | 6:CF:92:THR:OG1     | 1.98                     | 0.80              |
| 55:DA:3001:DOL:H432 | 55:DA:3001:DOL:C6   | 2.11                     | 0.79              |
| 55:DA:3001:DOL:O15  | 55:DA:3001:DOL:H212 | 1.82                     | 0.79              |
| 22:BA:2005:A:OP1    | 57:BA:3387:HOH:O    | 1.98                     | 0.79              |
| 11:CK:17:SER:O      | 11:CK:80:LYS:N      | 2.15                     | 0.79              |
| 20:AT:59:ASP:OD1    | 20:AT:76:LYS:NZ     | 2.15                     | 0.79              |
| 22:BA:622:G:OP2     | 57:BA:3293:HOH:O    | 2.00                     | 0.79              |
| 2:CB:103:ASN:ND2    | 2:CB:106:THR:OG1    | 2.15                     | 0.79              |
| 1:AA:1108:G:O6      | 57:AA:1862:HOH:O    | 1.98                     | 0.79              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 4:AD:163:GLU:OE2 | 4:AD:164:GLN:N    | 2.16                     | 0.79              |
| 22:DA:2261:C:C2  | 22:DA:2280:G:N2   | 2.51                     | 0.79              |
| 22:BA:58:G:OP1   | 41:BT:78:SER:CB   | 2.31                     | 0.79              |
| 22:DA:1091:G:O2' | 22:DA:1092:C:OP2  | 2.01                     | 0.79              |
| 22:DA:374:A:N6   | 22:DA:400:G:O2'   | 2.16                     | 0.79              |
| 39:DR:82:HIS:ND1 | 39:DR:82:HIS:O    | 2.16                     | 0.79              |
| 14:AN:64:CYS:SG  | 14:AN:67:THR:OG1  | 2.38                     | 0.79              |
| 22:BA:1925:C:H4' | 22:BA:1926:U:OP1  | 1.81                     | 0.79              |
| 22:DA:777:G:C2   | 22:DA:778:G:C8    | 2.71                     | 0.79              |
| 22:DA:2199:A:OP1 | 45:DX:37:ARG:NH1  | 2.15                     | 0.79              |
| 14:AN:90:ARG:NH1 | 14:AN:92:GLU:OE2  | 2.16                     | 0.79              |
| 22:BA:1379:U:C6  | 22:BA:1379:U:OP1  | 2.36                     | 0.79              |
| 22:DA:622:G:OP2  | 57:DA:3292:HOH:O  | 2.01                     | 0.79              |
| 23:DB:29:A:O2'   | 23:DB:58:A:N1     | 2.16                     | 0.79              |
| 24:DC:45:ASN:OD1 | 24:DC:46:ASN:N    | 2.16                     | 0.79              |
| 22:DA:488:G:N2   | 22:DA:493:G:O6    | 2.16                     | 0.78              |
| 1:AA:8:A:C6      | 4:AD:206:LYS:HB3  | 2.18                     | 0.78              |
| 16:AP:43:ALA:O   | 16:AP:44:SER:OG   | 2.00                     | 0.78              |
| 22:BA:1746:A:H2' | 22:BA:1747:U:C6   | 2.18                     | 0.78              |
| 22:BA:404:A:O2'  | 22:BA:405:U:OP2   | 2.01                     | 0.78              |
| 1:AA:684:U:O2'   | 11:AK:40:ASN:O    | 2.01                     | 0.78              |
| 22:DA:1141:U:OP2 | 31:DJ:65:THR:OG1  | 1.99                     | 0.78              |
| 35:DN:1:MET:H1   | 35:DN:1:MET:HE2   | 1.48                     | 0.78              |
| 50:D2:43:THR:OG1 | 50:D2:44:VAL:N    | 2.15                     | 0.78              |
| 22:DA:1627:G:C2  | 22:DA:1628:G:N7   | 2.52                     | 0.78              |
| 1:AA:652:U:O4    | 1:AA:752:G:O2'    | 2.00                     | 0.78              |
| 1:CA:195:A:OP1   | 20:CT:60:ARG:NH1  | 2.16                     | 0.78              |
| 1:CA:537:G:OP1   | 12:CL:110:ARG:NH2 | 2.16                     | 0.78              |
| 22:DA:1973:G:OP1 | 57:DA:3462:HOH:O  | 2.00                     | 0.78              |
| 22:DA:2579:C:OP1 | 57:DA:3538:HOH:O  | 2.02                     | 0.78              |
| 22:BA:1179:G:C4  | 22:BA:1180:U:H1'  | 2.19                     | 0.78              |
| 4:AD:125:VAL:O   | 4:AD:127:GLY:N    | 2.17                     | 0.78              |
| 22:DA:2576:G:O2' | 22:DA:2579:C:OP2  | 2.02                     | 0.77              |
| 22:BA:831:G:OP1  | 57:BA:3263:HOH:O  | 2.01                     | 0.77              |
| 1:AA:650:G:H2'   | 1:AA:651:C:H5'    | 1.64                     | 0.77              |
| 1:AA:1422:G:O3'  | 32:BK:49:ARG:NH2  | 2.17                     | 0.77              |
| 4:CD:192:SER:OG  | 4:CD:193:ALA:N    | 2.14                     | 0.77              |
| 4:AD:22:LYS:O    | 4:AD:24:GLY:N     | 2.17                     | 0.77              |
| 22:BA:481:G:C4   | 22:BA:507:A:C2    | 2.72                     | 0.77              |
| 1:CA:1499:A:OP2  | 57:CA:1884:HOH:O  | 2.00                     | 0.77              |
| 13:CM:40:ALA:O   | 13:CM:42:ASP:N    | 2.17                     | 0.77              |

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| Atom-1            | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 5:AE:99:ALA:O     | 5:AE:101:GLU:N      | 2.17                     | 0.77              |
| 28:BG:104:ASN:ND2 | 28:BG:114:ASP:OD1   | 2.17                     | 0.77              |
| 22:DA:856:G:N2    | 22:DA:922:C:C2      | 2.53                     | 0.77              |
| 22:BA:324:A:N6    | 22:BA:338:G:O2'     | 2.16                     | 0.77              |
| 22:DA:761:A:OP2   | 57:DA:3294:HOH:O    | 2.02                     | 0.77              |
| 1:CA:72:A:C6      | 1:CA:73:C:N4        | 2.52                     | 0.77              |
| 22:BA:2831:G:OP1  | 25:BD:56:LYS:NZ     | 2.17                     | 0.77              |
| 1:CA:890:G:O2'    | 1:CA:906:A:N6       | 2.17                     | 0.77              |
| 29:DH:1:MET:SD    | 29:DH:27:ARG:NH1    | 2.58                     | 0.77              |
| 37:DP:65:SER:O    | 37:DP:67:GLY:N      | 2.18                     | 0.77              |
| 1:AA:1018:G:C2    | 1:AA:1019:A:C8      | 2.73                     | 0.76              |
| 2:AB:50:PHE:HA    | 2:AB:213:TYR:OH     | 1.85                     | 0.76              |
| 22:BA:2287:A:OP1  | 49:B1:30:LYS:NZ     | 2.18                     | 0.76              |
| 22:DA:1515:A:O2'  | 22:DA:1556:C:O2'    | 2.02                     | 0.76              |
| 22:DA:2507:C:OP1  | 57:DA:3708:HOH:O    | 2.02                     | 0.76              |
| 1:AA:1278:G:H4'   | 1:AA:1279:G:C8      | 2.21                     | 0.76              |
| 7:AG:99:LEU:O     | 7:AG:102:ARG:N      | 2.17                     | 0.76              |
| 1:AA:31:G:O2'     | 1:AA:48:C:N4        | 2.18                     | 0.76              |
| 1:AA:993:G:O2'    | 1:AA:994:A:N7       | 2.18                     | 0.76              |
| 22:BA:1922:G:N2   | 22:BA:1923:U:H1'    | 2.00                     | 0.76              |
| 29:DH:53:GLU:O    | 29:DH:55:GLU:N      | 2.19                     | 0.76              |
| 1:CA:718:A:C8     | 1:CA:719:C:C5       | 2.74                     | 0.76              |
| 22:DA:332:A:O2'   | 22:DA:334:C:OP2     | 2.03                     | 0.76              |
| 29:DH:45:GLU:O    | 29:DH:49:ALA:N      | 2.19                     | 0.76              |
| 5:AE:69:ARG:O     | 5:AE:71:MET:N       | 2.18                     | 0.76              |
| 40:BS:29:VAL:HG13 | 40:BS:55:ILE:HD11   | 1.68                     | 0.76              |
| 22:DA:1009:A:N3   | 22:DA:1153:C:O2'    | 2.18                     | 0.76              |
| 22:DA:2504:U:C4   | 55:DA:3001:DOL:H161 | 2.21                     | 0.76              |
| 24:DC:258:ARG:NH1 | 24:DC:264:ASP:OD2   | 2.18                     | 0.76              |
| 22:BA:2305:U:C2   | 27:BF:151:GLY:HA3   | 2.20                     | 0.76              |
| 2:AB:23:TRP:CH2   | 2:AB:25:PRO:HA      | 2.21                     | 0.76              |
| 22:BA:2271:G:O6   | 57:BA:3514:HOH:O    | 2.04                     | 0.76              |
| 22:BA:276:U:O2'   | 22:BA:278:A:N7      | 2.19                     | 0.76              |
| 49:D1:15:ALA:O    | 49:D1:17:THR:N      | 2.19                     | 0.76              |
| 22:DA:444:C:OP1   | 26:DE:40:ARG:NH1    | 2.19                     | 0.76              |
| 1:AA:792:A:H4'    | 1:AA:793:U:O5'      | 1.85                     | 0.76              |
| 1:CA:527:G:C2     | 1:CA:528:C:C6       | 2.74                     | 0.76              |
| 1:CA:567:G:O2'    | 57:CA:1705:HOH:O    | 2.04                     | 0.76              |
| 2:CB:193:PRO:O    | 2:CB:195:GLY:N      | 2.18                     | 0.76              |
| 22:DA:1340:U:C5   | 22:DA:1603:A:C8     | 2.75                     | 0.76              |
| 22:DA:1677:A:N7   | 57:DA:3765:HOH:O    | 2.17                     | 0.76              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AA:111:G:C6     | 1:AA:330:C:N4     | 2.53                     | 0.75              |
| 2:CB:58:ASN:ND2   | 2:CB:220:THR:O    | 2.19                     | 0.75              |
| 13:CM:13:LYS:O    | 13:CM:14:HIS:ND1  | 2.19                     | 0.75              |
| 21:AU:35:ARG:O    | 21:AU:37:PHE:N    | 2.18                     | 0.75              |
| 22:BA:1474:U:H2'  | 22:BA:1475:G:H5'  | 1.68                     | 0.75              |
| 29:BH:91:PHE:O    | 1:CA:55:A:C6      | 2.40                     | 0.75              |
| 21:CU:51:SER:O    | 21:CU:53:VAL:N    | 2.19                     | 0.75              |
| 1:AA:208:U:C5     | 1:AA:210:C:C4     | 2.75                     | 0.75              |
| 1:AA:338:A:N1     | 1:AA:351:G:O6     | 2.18                     | 0.75              |
| 1:CA:1124:G:O2'   | 1:CA:1145:A:N6    | 2.18                     | 0.75              |
| 17:CQ:69:LYS:O    | 17:CQ:70:THR:OG1  | 2.04                     | 0.75              |
| 22:DA:2286:G:H4'  | 22:DA:2287:A:O5'  | 1.86                     | 0.75              |
| 24:DC:70:ASN:O    | 24:DC:72:ASP:N    | 2.20                     | 0.75              |
| 29:DH:124:THR:OG1 | 29:DH:125:THR:N   | 2.17                     | 0.75              |
| 2:AB:63:ARG:O     | 2:AB:64:LYS:HB2   | 1.87                     | 0.75              |
| 22:BA:2448:A:OP2  | 57:BA:3686:HOH:O  | 2.03                     | 0.75              |
| 6:AF:91:ARG:C     | 6:AF:92:THR:HG1   | 1.89                     | 0.75              |
| 22:BA:653:U:OP2   | 22:BA:653:U:C6    | 2.38                     | 0.75              |
| 34:BM:42:THR:HG22 | 34:BM:93:VAL:HG12 | 1.67                     | 0.75              |
| 1:CA:1181:G:O2'   | 1:CA:1182:G:N7    | 2.19                     | 0.75              |
| 4:AD:11:LEU:HD22  | 4:AD:63:ARG:HD3   | 1.69                     | 0.75              |
| 22:BA:731:C:OP2   | 57:BA:3697:HOH:O  | 2.04                     | 0.75              |
| 5:CE:41:ASP:OD1   | 5:CE:42:GLY:N     | 2.20                     | 0.75              |
| 22:BA:1464:G:O6   | 57:BA:3642:HOH:O  | 2.05                     | 0.75              |
| 1:CA:734:G:C2     | 1:CA:735:C:C6     | 2.74                     | 0.75              |
| 1:CA:684:U:O2'    | 11:CK:40:ASN:O    | 2.04                     | 0.75              |
| 22:DA:49:A:C8     | 22:DA:51:G:N2     | 2.55                     | 0.75              |
| 22:DA:788:A:OP1   | 22:DA:791:C:N4    | 2.19                     | 0.75              |
| 46:DY:11:VAL:O    | 46:DY:15:ASN:ND2  | 2.18                     | 0.75              |
| 22:BA:1509:A:O2'  | 22:BA:1510:G:P    | 2.45                     | 0.75              |
| 42:DU:9:ASP:OD2   | 42:DU:10:GLU:N    | 2.20                     | 0.75              |
| 5:AE:104:GLY:O    | 5:AE:105:ILE:HG22 | 1.87                     | 0.75              |
| 16:AP:42:ILE:O    | 16:AP:44:SER:N    | 2.20                     | 0.75              |
| 53:B5:50:ILE:C    | 53:B5:52:PRO:HD3  | 2.06                     | 0.75              |
| 11:AK:13:ARG:NE   | 22:BA:2142:A:OP1  | 2.20                     | 0.75              |
| 22:BA:617:G:N7    | 57:BA:3291:HOH:O  | 2.19                     | 0.75              |
| 1:AA:82:G:N2      | 1:AA:89:U:OP1     | 2.19                     | 0.74              |
| 22:BA:2711:A:OP2  | 57:BA:3550:HOH:O  | 2.05                     | 0.74              |
| 22:DA:2407:A:OP1  | 57:DA:3560:HOH:O  | 2.04                     | 0.74              |
| 22:DA:225:C:N4    | 22:DA:419:U:O2'   | 2.18                     | 0.74              |
| 1:AA:251:G:C6     | 1:AA:266:G:C6     | 2.75                     | 0.74              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 22:DA:1266:G:O2'   | 22:DA:2012:G:O6     | 2.03                     | 0.74              |
| 22:DA:2127:G:O2'   | 22:DA:2173:A:N3     | 2.20                     | 0.74              |
| 1:AA:131:A:H2'     | 1:AA:132:C:C6       | 2.23                     | 0.74              |
| 32:BK:78:ARG:NH1   | 37:BP:71:GLU:OE2    | 2.20                     | 0.74              |
| 2:CB:87:CYS:O      | 2:CB:89:GLN:N       | 2.20                     | 0.74              |
| 22:BA:1378:A:O2'   | 22:BA:1380:G:OP2    | 2.05                     | 0.74              |
| 29:BH:117:LEU:HD11 | 29:BH:122:LEU:HD12  | 1.69                     | 0.74              |
| 22:DA:2550:G:OP1   | 57:DA:3720:HOH:O    | 2.05                     | 0.74              |
| 22:DA:27:G:O2'     | 22:DA:28:A:OP2      | 2.05                     | 0.74              |
| 1:AA:411:A:OP1     | 4:AD:26:ARG:NH2     | 2.20                     | 0.74              |
| 22:BA:2125:G:N3    | 22:BA:2173:A:N6     | 2.36                     | 0.74              |
| 29:BH:88:GLY:O     | 29:BH:125:THR:OG1   | 2.04                     | 0.74              |
| 22:BA:1179:G:C6    | 22:BA:1180:U:C2     | 2.74                     | 0.74              |
| 22:BA:1921:G:C2    | 22:BA:1922:G:C8     | 2.76                     | 0.74              |
| 29:BH:123:ARG:C    | 29:BH:124:THR:HG23  | 2.06                     | 0.74              |
| 33:BL:87:GLY:O     | 33:BL:89:VAL:N      | 2.21                     | 0.74              |
| 1:CA:533:A:OP1     | 57:CA:1763:HOH:O    | 2.05                     | 0.74              |
| 22:DA:306:U:O2     | 22:DA:312:G:N2      | 2.21                     | 0.74              |
| 11:AK:29:ASN:OD1   | 11:AK:30:THR:N      | 2.21                     | 0.74              |
| 22:DA:2063:C:H4'   | 55:DA:3001:DOL:H343 | 1.69                     | 0.74              |
| 22:DA:998:C:OP2    | 38:DQ:58:ARG:NH2    | 2.20                     | 0.74              |
| 14:AN:61:ARG:O     | 14:AN:62:ASN:HB2    | 1.86                     | 0.74              |
| 51:B3:31:HIS:CD2   | 51:B3:32:ILE:HG13   | 2.22                     | 0.74              |
| 4:CD:95:GLU:OE2    | 4:CD:100:ASN:ND2    | 2.20                     | 0.74              |
| 1:AA:1225:A:H2'    | 1:AA:1226:C:C5      | 2.22                     | 0.74              |
| 24:BC:143:ASN:OD1  | 24:BC:152:GLY:HA3   | 1.87                     | 0.74              |
| 1:AA:568:G:C2      | 1:AA:569:C:C5       | 2.76                     | 0.73              |
| 1:AA:667:G:H4'     | 15:AO:51:HIS:ND1    | 2.03                     | 0.73              |
| 13:AM:82:ASP:OD1   | 27:BF:112:ARG:NH2   | 2.21                     | 0.73              |
| 22:BA:1669:A:OP2   | 57:BA:3723:HOH:O    | 2.06                     | 0.73              |
| 14:CN:21:PHE:O     | 14:CN:23:LYS:N      | 2.21                     | 0.73              |
| 35:DN:90:ARG:CZ    | 35:DN:116:VAL:HG11  | 2.18                     | 0.73              |
| 17:AQ:81:LYS:O     | 17:AQ:83:VAL:N      | 2.22                     | 0.73              |
| 22:BA:1179:G:C5    | 22:BA:1180:U:H1'    | 2.22                     | 0.73              |
| 1:CA:1147:C:O2     | 9:CI:18:ARG:NH2     | 2.21                     | 0.73              |
| 4:AD:95:GLU:OE2    | 4:AD:104:ARG:NH1    | 2.20                     | 0.73              |
| 22:DA:561:G:HO2'   | 38:DQ:45:TYR:HH     | 1.32                     | 0.73              |
| 4:AD:11:LEU:CD2    | 4:AD:63:ARG:HD3     | 2.19                     | 0.73              |
| 21:AU:36:GLU:O     | 21:AU:37:PHE:HB2    | 1.86                     | 0.73              |
| 27:BF:158:THR:O    | 57:BF:201:HOH:O     | 2.05                     | 0.73              |
| 22:BA:997:G:OP1    | 38:BQ:92:ARG:HG2    | 1.88                     | 0.73              |

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| Atom-1            | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 22:BA:2506:U:C5   | 55:BA:3001:DOL:H422 | 2.23                     | 0.73              |
| 22:BA:58:G:OP1    | 41:BT:78:SER:HB3    | 1.88                     | 0.73              |
| 46:BY:61:ALA:O    | 46:BY:63:ALA:N      | 2.21                     | 0.73              |
| 22:DA:1153:C:OP1  | 57:DA:3359:HOH:O    | 2.07                     | 0.73              |
| 22:DA:1475:G:O2'  | 22:DA:1476:U:OP1    | 2.07                     | 0.73              |
| 22:DA:1715:G:O2'  | 22:DA:1743:G:O6     | 2.07                     | 0.73              |
| 22:BA:455:C:N3    | 22:BA:472:A:H2'     | 2.04                     | 0.73              |
| 22:DA:684:G:C2    | 22:DA:794:A:C2      | 2.77                     | 0.73              |
| 25:DD:56:LYS:O    | 25:DD:58:ASN:N      | 2.22                     | 0.73              |
| 1:AA:844:G:C6     | 1:AA:846:G:O2'      | 2.42                     | 0.73              |
| 22:BA:1061:U:HO2' | 22:BA:1062:G:P      | 2.12                     | 0.73              |
| 22:BA:2189:U:H2'  | 22:BA:2190:G:C8     | 2.24                     | 0.73              |
| 22:DA:1342:A:OP2  | 57:DA:3711:HOH:O    | 2.05                     | 0.73              |
| 22:DA:1604:C:OP1  | 57:DA:3403:HOH:O    | 2.07                     | 0.73              |
| 22:DA:503:A:C2    | 22:DA:506:G:C4      | 2.77                     | 0.73              |
| 14:AN:46:LEU:O    | 14:AN:48:LEU:N      | 2.22                     | 0.72              |
| 17:AQ:16:LYS:C    | 17:AQ:17:MET:SD     | 2.68                     | 0.72              |
| 22:BA:730:A:P     | 57:BA:3695:HOH:O    | 2.38                     | 0.72              |
| 22:BA:84:A:N1     | 22:BA:98:G:O2'      | 2.21                     | 0.72              |
| 39:BR:39:LEU:HA   | 39:BR:49:ILE:CG2    | 2.19                     | 0.72              |
| 26:DE:21:ARG:NH1  | 26:DE:103:GLY:O     | 2.21                     | 0.72              |
| 1:AA:1074:G:OP1   | 5:AE:69:ARG:NH2     | 2.22                     | 0.72              |
| 1:CA:1525:G:O6    | 57:CA:1892:HOH:O    | 2.05                     | 0.72              |
| 1:CA:679:C:O2     | 1:CA:712:A:C2       | 2.42                     | 0.72              |
| 10:CJ:87:LEU:HD13 | 10:CJ:88:MET:N      | 2.04                     | 0.72              |
| 1:AA:984:C:N4     | 57:AA:1838:HOH:O    | 2.21                     | 0.72              |
| 22:BA:245:G:O6    | 51:B3:8:ARG:HD3     | 1.88                     | 0.72              |
| 1:CA:552:U:C4     | 1:CA:553:A:N7       | 2.57                     | 0.72              |
| 42:DU:36:VAL:O    | 42:DU:38:GLY:N      | 2.22                     | 0.72              |
| 1:AA:203:G:N2     | 1:AA:215:C:C2       | 2.58                     | 0.72              |
| 22:BA:1182:G:H2'  | 22:BA:1183:U:O4'    | 1.89                     | 0.72              |
| 23:BB:8:C:O3'     | 36:BO:25:ARG:NH1    | 2.21                     | 0.72              |
| 22:DA:1935:G:H1'  | 22:DA:1964:G:N2     | 2.03                     | 0.72              |
| 22:DA:2684:U:O4'  | 32:DK:70:ARG:NH1    | 2.22                     | 0.72              |
| 14:AN:64:CYS:HG   | 14:AN:67:THR:HG1    | 1.34                     | 0.72              |
| 22:BA:1916:A:H2'  | 22:BA:1917:U:C1'    | 2.20                     | 0.72              |
| 31:BJ:81:ILE:HG23 | 31:BJ:82:GLY:N      | 2.04                     | 0.72              |
| 22:DA:583:G:C6    | 22:DA:584:C:C4      | 2.78                     | 0.72              |
| 35:DN:106:ASP:O   | 35:DN:108:ALA:N     | 2.22                     | 0.72              |
| 1:CA:1385:G:N7    | 57:CA:1874:HOH:O    | 2.22                     | 0.72              |
| 5:CE:80:THR:OG1   | 5:CE:122:ASN:ND2    | 2.22                     | 0.72              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:DA:116:C:O2'   | 22:DA:126:A:O2'   | 2.05                     | 0.72              |
| 22:DA:981:A:OP2   | 22:DA:982:C:N4    | 2.22                     | 0.72              |
| 22:BA:193:U:OP2   | 57:BA:3741:HOH:O  | 2.08                     | 0.72              |
| 22:BA:626:A:H2'   | 33:BL:78:ARG:NH1  | 2.03                     | 0.72              |
| 41:BT:49:LYS:N    | 41:BT:49:LYS:HD3  | 2.05                     | 0.72              |
| 1:CA:734:G:N3     | 1:CA:735:C:C6     | 2.57                     | 0.72              |
| 27:BF:36:LEU:HD21 | 27:BF:99:PHE:CE1  | 2.25                     | 0.72              |
| 19:CS:4:SER:O     | 19:CS:5:LEU:HB2   | 1.90                     | 0.72              |
| 22:DA:2057:G:OP2  | 57:DA:3485:HOH:O  | 2.07                     | 0.72              |
| 22:DA:2355:G:OP1  | 44:DW:25:ARG:NH2  | 2.23                     | 0.72              |
| 16:AP:22:ALA:HA   | 16:AP:33:ILE:HG13 | 1.72                     | 0.72              |
| 1:AA:178:C:OP2    | 20:AT:60:ARG:NH2  | 2.23                     | 0.72              |
| 22:BA:495:G:H1'   | 40:BS:57:ASN:OD1  | 1.90                     | 0.72              |
| 5:CE:101:GLU:CD   | 5:CE:101:GLU:O    | 2.28                     | 0.72              |
| 22:DA:1469:A:H2'  | 22:DA:1470:A:C8   | 2.25                     | 0.72              |
| 22:DA:79:C:O2'    | 22:DA:346:A:N3    | 2.21                     | 0.72              |
| 1:CA:1219:A:N6    | 1:CA:1220:G:O6    | 2.23                     | 0.72              |
| 4:CD:100:ASN:OD1  | 4:CD:111:ARG:NH1  | 2.21                     | 0.72              |
| 2:AB:82:ASP:O     | 2:AB:85:LEU:N     | 2.23                     | 0.71              |
| 22:DA:616:A:H4'   | 26:DE:101:TYR:CZ  | 2.24                     | 0.71              |
| 1:AA:1222:G:O6    | 57:AA:1837:HOH:O  | 2.08                     | 0.71              |
| 24:BC:230:HIS:CD2 | 24:BC:247:PRO:HA  | 2.24                     | 0.71              |
| 1:CA:374:A:H5''   | 1:CA:452:A:N1     | 2.05                     | 0.71              |
| 22:DA:2622:U:O2'  | 22:DA:2825:G:N7   | 2.22                     | 0.71              |
| 9:AI:49:ARG:NH2   | 9:AI:52:LEU:O     | 2.23                     | 0.71              |
| 5:CE:132:ASN:O    | 5:CE:136:VAL:HG12 | 1.91                     | 0.71              |
| 16:AP:50:THR:O    | 16:AP:50:THR:HG22 | 1.90                     | 0.71              |
| 21:AU:34:ARG:CZ   | 21:AU:35:ARG:HB2  | 2.20                     | 0.71              |
| 22:BA:1653:G:H3'  | 35:BN:2:ARG:HG3   | 1.72                     | 0.71              |
| 37:BP:54:GLY:O    | 37:BP:57:SER:OG   | 2.07                     | 0.71              |
| 22:DA:1335:C:N4   | 57:DA:3392:HOH:O  | 2.23                     | 0.71              |
| 29:DH:31:VAL:HB   | 29:DH:32:PRO:CD   | 2.20                     | 0.71              |
| 1:AA:64:G:C8      | 1:AA:99:C:N4      | 2.58                     | 0.71              |
| 25:BD:103:ASP:O   | 25:BD:105:LYS:N   | 2.23                     | 0.71              |
| 22:DA:698:C:O2'   | 22:DA:734:A:N6    | 2.23                     | 0.71              |
| 1:AA:109:A:H2'    | 1:AA:326:G:N2     | 2.06                     | 0.71              |
| 22:BA:1917:U:C4   | 22:BA:1918:A:C6   | 2.78                     | 0.71              |
| 22:BA:500:G:N2    | 22:BA:502:A:H3'   | 2.06                     | 0.71              |
| 49:D1:5:ILE:O     | 49:D1:28:ARG:NH1  | 2.23                     | 0.71              |
| 1:AA:154:U:C2     | 1:AA:168:G:N2     | 2.58                     | 0.71              |
| 46:BY:6:LEU:O     | 46:BY:60:LYS:NZ   | 2.24                     | 0.71              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 22:DA:1259:G:H2'   | 22:DA:1260:A:C8     | 2.25                     | 0.71              |
| 22:DA:910:A:N3     | 22:DA:2264:C:O2'    | 2.23                     | 0.71              |
| 22:BA:1385:A:H1'   | 22:BA:1386:C:C6     | 2.26                     | 0.71              |
| 39:BR:49:ILE:HG22  | 39:BR:53:PHE:CA     | 2.21                     | 0.71              |
| 22:DA:2061:G:O6    | 55:DA:3001:DOL:H162 | 1.90                     | 0.71              |
| 22:DA:58:G:N3      | 22:DA:70:G:N2       | 2.39                     | 0.71              |
| 22:DA:1187:G:H5''  | 39:DR:83:TYR:CE2    | 2.26                     | 0.71              |
| 2:AB:151:ILE:HD12  | 2:AB:154:MET:SD     | 2.31                     | 0.70              |
| 22:BA:1779:U:C5    | 22:BA:1784:A:N7     | 2.58                     | 0.70              |
| 39:BR:48:LYS:HG2   | 39:BR:48:LYS:O      | 1.91                     | 0.70              |
| 39:BR:49:ILE:HG22  | 39:BR:53:PHE:N      | 2.06                     | 0.70              |
| 1:CA:1108:G:O6     | 57:CA:1858:HOH:O    | 2.05                     | 0.70              |
| 4:CD:26:ARG:HG3    | 4:CD:27:ALA:N       | 2.06                     | 0.70              |
| 22:DA:126:A:C2     | 50:D2:18:PHE:CE2    | 2.79                     | 0.70              |
| 22:DA:1251:C:OP2   | 38:DQ:6:ARG:NH2     | 2.24                     | 0.70              |
| 22:DA:300:A:HO2'   | 22:DA:318:C:HO2'    | 1.33                     | 0.70              |
| 22:BA:2555:U:C5    | 22:BA:2556:C:C2     | 2.78                     | 0.70              |
| 4:AD:174:ASP:OD2   | 4:AD:176:GLY:N      | 2.24                     | 0.70              |
| 5:AE:82:GLN:NE2    | 5:AE:150:PRO:HD3    | 2.06                     | 0.70              |
| 22:BA:2291:U:H2'   | 22:BA:2292:U:C6     | 2.26                     | 0.70              |
| 55:DA:3001:DOL:C48 | 55:DA:3001:DOL:C46  | 2.58                     | 0.70              |
| 26:DE:21:ARG:O     | 26:DE:114:ARG:NH2   | 2.24                     | 0.70              |
| 22:BA:1604:C:OP2   | 57:BA:3414:HOH:O    | 2.08                     | 0.70              |
| 11:AK:76:GLU:C     | 22:BA:2141:G:OP1    | 2.29                     | 0.70              |
| 22:BA:2189:U:H2'   | 22:BA:2190:G:C1'    | 2.21                     | 0.70              |
| 22:BA:265:A:N1     | 22:BA:427:U:O2'     | 2.24                     | 0.70              |
| 1:CA:1124:G:N2     | 1:CA:1127:G:C2      | 2.60                     | 0.70              |
| 12:CL:57:LEU:O     | 12:CL:60:GLY:N      | 2.23                     | 0.70              |
| 1:CA:1302:C:C4     | 13:CM:17:ILE:HD13   | 2.26                     | 0.70              |
| 1:AA:1406:U:C5     | 1:AA:1407:C:C5      | 2.79                     | 0.70              |
| 31:BJ:114:LEU:HG   | 31:BJ:118:MET:HE3   | 1.72                     | 0.70              |
| 42:BU:12:ILE:HG21  | 42:BU:80:ALA:HB2    | 1.73                     | 0.70              |
| 22:DA:134:G:C2     | 22:DA:146:A:C2      | 2.79                     | 0.70              |
| 22:BA:181:A:H2'    | 22:BA:182:A:C8      | 2.26                     | 0.70              |
| 22:BA:2192:U:H2'   | 22:BA:2193:G:H5'    | 1.72                     | 0.70              |
| 22:BA:620:G:H4'    | 22:BA:621:A:O5'     | 1.91                     | 0.70              |
| 27:BF:127:ASN:OD1  | 27:BF:157:THR:HA    | 1.92                     | 0.70              |
| 22:DA:2004:G:OP1   | 57:DA:3798:HOH:O    | 2.09                     | 0.70              |
| 22:DA:733:G:OP2    | 57:DA:3295:HOH:O    | 2.09                     | 0.70              |
| 17:AQ:69:LYS:O     | 17:AQ:70:THR:CB     | 2.39                     | 0.70              |
| 1:CA:811:C:O2'     | 1:CA:901:A:N1       | 2.24                     | 0.70              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 21:CU:18:ARG:O    | 21:CU:21:ARG:N     | 2.24                     | 0.70              |
| 41:DT:17:SER:O    | 41:DT:19:LYS:N     | 2.24                     | 0.70              |
| 43:DV:51:GLN:HB3  | 43:DV:56:PHE:CG    | 2.27                     | 0.70              |
| 11:AK:26:SER:O    | 11:AK:28:ASN:N     | 2.24                     | 0.70              |
| 22:BA:1923:U:C2'  | 22:BA:1924:C:H5'   | 2.19                     | 0.70              |
| 22:BA:2258:C:O2'  | 22:BA:2427:C:OP2   | 2.10                     | 0.70              |
| 29:BH:94:ILE:HG22 | 29:BH:99:ILE:HG13  | 1.72                     | 0.70              |
| 1:CA:977:A:N3     | 1:CA:977:A:H3'     | 2.07                     | 0.70              |
| 2:CB:15:HIS:O     | 2:CB:17:GLY:N      | 2.25                     | 0.70              |
| 12:AL:44:LYS:CB   | 12:AL:45:PRO:CD    | 2.70                     | 0.70              |
| 22:BA:2191:A:C6   | 22:BA:2192:U:O4    | 2.45                     | 0.70              |
| 22:BA:2308:G:O6   | 22:BA:2311:A:N7    | 2.24                     | 0.70              |
| 39:BR:49:ILE:HB   | 39:BR:52:PRO:C     | 2.11                     | 0.70              |
| 22:DA:192:C:OP1   | 57:DA:3737:HOH:O   | 2.09                     | 0.70              |
| 22:DA:1993:U:H4'  | 25:DD:133:THR:HG22 | 1.73                     | 0.70              |
| 22:DA:1649:G:C6   | 22:DA:2009:A:C6    | 2.80                     | 0.70              |
| 22:DA:2415:G:C6   | 22:DA:2416:C:C4    | 2.80                     | 0.70              |
| 22:DA:526:A:N6    | 22:DA:2626:C:H4'   | 2.06                     | 0.70              |
| 22:BA:1141:U:H4'  | 22:BA:1142:A:O4'   | 1.92                     | 0.70              |
| 22:DA:2816:G:N3   | 22:DA:2883:A:O2'   | 2.22                     | 0.70              |
| 1:AA:1304:G:OP2   | 57:AA:1797:HOH:O   | 2.10                     | 0.69              |
| 20:AT:43:ASP:OD1  | 20:AT:46:ALA:N     | 2.24                     | 0.69              |
| 22:BA:194:G:N7    | 57:BA:3758:HOH:O   | 2.25                     | 0.69              |
| 22:BA:528:A:C2    | 22:BA:2043:C:H5'   | 2.27                     | 0.69              |
| 32:DK:34:GLY:O    | 32:DK:36:GLY:N     | 2.25                     | 0.69              |
| 39:DR:49:ILE:HG22 | 39:DR:54:VAL:N     | 2.07                     | 0.69              |
| 1:AA:144:G:C4     | 1:AA:179:A:C2      | 2.79                     | 0.69              |
| 11:AK:76:GLU:O    | 11:AK:77:TYR:CD1   | 2.45                     | 0.69              |
| 35:BN:65:LEU:HD11 | 35:BN:69:ARG:NH2   | 2.05                     | 0.69              |
| 1:CA:376:G:H5'    | 16:CP:5:ARG:HB3    | 1.74                     | 0.69              |
| 1:CA:496:A:C2     | 1:CA:497:G:C5      | 2.80                     | 0.69              |
| 1:CA:582:C:N3     | 1:CA:760:G:C6      | 2.60                     | 0.69              |
| 5:CE:155:ALA:HB1  | 8:CH:66:PHE:CD2    | 2.26                     | 0.69              |
| 22:DA:2134:A:OP2  | 22:DA:2157:G:N2    | 2.24                     | 0.69              |
| 22:DA:864:G:C6    | 22:DA:865:C:N4     | 2.60                     | 0.69              |
| 4:AD:174:ASP:OD2  | 4:AD:177:LYS:N     | 2.25                     | 0.69              |
| 22:BA:1073:A:H3'  | 22:BA:1074:G:H5'   | 1.74                     | 0.69              |
| 22:BA:370:G:OP2   | 57:BA:3561:HOH:O   | 2.09                     | 0.69              |
| 22:DA:118:A:C8    | 22:DA:119:A:C8     | 2.80                     | 0.69              |
| 22:DA:1809:A:H2'  | 22:DA:1810:A:C8    | 2.27                     | 0.69              |
| 11:AK:102:ALA:O   | 11:AK:104:GLY:N    | 2.26                     | 0.69              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:BA:125:A:OP2   | 50:B2:19:ARG:NH2  | 2.25                     | 0.69              |
| 23:BB:91:C:OP2    | 34:BM:18:ARG:HG2  | 1.91                     | 0.69              |
| 1:CA:495:A:C2     | 1:CA:496:A:N6     | 2.60                     | 0.69              |
| 22:DA:1509:A:O2'  | 22:DA:1510:G:P    | 2.51                     | 0.69              |
| 1:AA:692:U:O2'    | 1:AA:694:A:N7     | 2.17                     | 0.69              |
| 28:BG:155:GLU:OE2 | 28:BG:158:LYS:N   | 2.26                     | 0.69              |
| 22:DA:1358:G:O2'  | 22:DA:1359:A:H5'  | 1.92                     | 0.69              |
| 22:DA:1544:A:N1   | 22:DA:1545:A:C2   | 2.61                     | 0.69              |
| 28:DG:111:HIS:O   | 28:DG:111:HIS:ND1 | 2.26                     | 0.69              |
| 1:AA:484:G:H4'    | 1:AA:485:U:OP1    | 1.92                     | 0.69              |
| 22:BA:747:U:C5    | 22:BA:2613:U:C5   | 2.81                     | 0.69              |
| 22:DA:1088:A:N6   | 30:DI:135:SER:OG  | 2.24                     | 0.69              |
| 22:DA:2032:G:H1'  | 25:DD:150:GLN:NE2 | 2.06                     | 0.69              |
| 22:DA:2821:A:OP2  | 25:DD:115:GLY:N   | 2.26                     | 0.69              |
| 22:DA:46:G:C2     | 22:DA:47:C:C5     | 2.79                     | 0.69              |
| 2:AB:21:ARG:HA    | 2:AB:21:ARG:CZ    | 2.22                     | 0.69              |
| 4:AD:120:HIS:O    | 4:AD:122:ALA:N    | 2.26                     | 0.69              |
| 33:BL:82:LEU:HD23 | 33:BL:83:ALA:N    | 2.07                     | 0.69              |
| 1:CA:533:A:O2'    | 1:CA:535:A:OP2    | 2.11                     | 0.69              |
| 1:CA:1348:U:H4'   | 9:CI:122:ARG:HG3  | 1.74                     | 0.69              |
| 22:DA:1208:C:C4   | 22:DA:1209:U:C4   | 2.81                     | 0.69              |
| 25:DD:151:THR:O   | 25:DD:152:PRO:C   | 2.30                     | 0.69              |
| 1:CA:688:G:O2'    | 1:CA:704:A:N1     | 2.21                     | 0.69              |
| 22:DA:152:A:C2    | 22:DA:175:G:C2    | 2.81                     | 0.69              |
| 22:DA:2115:G:O2'  | 22:DA:2117:A:N6   | 2.25                     | 0.69              |
| 22:DA:39:G:C6     | 22:DA:40:U:C4     | 2.81                     | 0.69              |
| 22:DA:763:G:OP1   | 57:DA:3691:HOH:O  | 2.11                     | 0.69              |
| 22:BA:997:G:OP1   | 38:BQ:92:ARG:CG   | 2.41                     | 0.69              |
| 9:CI:12:ARG:NH1   | 9:CI:107:ASP:OD2  | 2.26                     | 0.69              |
| 22:DA:608:A:H2'   | 22:DA:609:A:C8    | 2.27                     | 0.69              |
| 22:DA:740:C:H5'   | 22:DA:1784:A:H3'  | 1.75                     | 0.69              |
| 35:DN:1:MET:CE    | 35:DN:1:MET:H1    | 2.05                     | 0.69              |
| 2:AB:87:CYS:O     | 2:AB:89:GLN:N     | 2.26                     | 0.69              |
| 22:BA:2191:A:H2'  | 22:BA:2192:U:C6   | 2.28                     | 0.69              |
| 1:CA:1095:U:OP2   | 57:CA:1858:HOH:O  | 2.09                     | 0.69              |
| 1:CA:66:A:C6      | 1:CA:67:C:C5      | 2.81                     | 0.69              |
| 1:CA:875:U:O2'    | 8:CH:15:ARG:NH1   | 2.26                     | 0.69              |
| 22:DA:362:A:C5    | 22:DA:363:G:C8    | 2.81                     | 0.69              |
| 22:DA:377:G:C6    | 22:DA:378:C:C4    | 2.81                     | 0.69              |
| 1:AA:858:G:O6     | 57:AA:1824:HOH:O  | 2.09                     | 0.69              |
| 22:BA:1494:A:C2'  | 22:BA:1495:A:O5'  | 2.41                     | 0.69              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:BA:686:U:H2'   | 22:BA:788:A:N1     | 2.08                     | 0.69              |
| 37:BP:52:ASN:O    | 37:BP:53:ARG:HG2   | 1.93                     | 0.69              |
| 1:CA:8:A:C6       | 4:CD:206:LYS:HB3   | 2.28                     | 0.69              |
| 22:DA:2886:A:C2   | 22:DA:2887:A:H1'   | 2.28                     | 0.69              |
| 22:DA:414:C:O2    | 22:DA:2410:G:N2    | 2.25                     | 0.69              |
| 22:DA:53:A:N7     | 22:DA:54:G:C4      | 2.61                     | 0.69              |
| 11:AK:38:GLN:O    | 11:AK:40:ASN:ND2   | 2.26                     | 0.68              |
| 12:AL:24:LEU:O    | 12:AL:25:GLU:C     | 2.30                     | 0.68              |
| 13:AM:64:VAL:HG12 | 13:AM:64:VAL:O     | 1.93                     | 0.68              |
| 1:CA:1004:A:O2'   | 1:CA:1036:A:N1     | 2.26                     | 0.68              |
| 22:DA:1773:A:N7   | 22:DA:1829:A:H1'   | 2.08                     | 0.68              |
| 22:DA:732:C:OP2   | 57:DA:3297:HOH:O   | 2.11                     | 0.68              |
| 32:DK:76:VAL:HG12 | 37:DP:73:VAL:HG22  | 1.74                     | 0.68              |
| 1:AA:254:G:OP1    | 17:AQ:70:THR:HB    | 1.92                     | 0.68              |
| 5:AE:137:VAL:O    | 5:AE:138:ARG:HB2   | 1.93                     | 0.68              |
| 16:AP:46:LYS:HD3  | 16:AP:47:GLU:N     | 2.07                     | 0.68              |
| 22:BA:1433:A:O2'  | 22:BA:1434:A:H5'   | 1.93                     | 0.68              |
| 22:BA:752:A:C2    | 22:BA:1781:U:C2    | 2.82                     | 0.68              |
| 22:BA:2448:A:OP2  | 57:BA:3687:HOH:O   | 2.10                     | 0.68              |
| 24:BC:71:LYS:NZ   | 24:BC:98:ASP:OD2   | 2.26                     | 0.68              |
| 29:BH:117:LEU:O   | 29:BH:121:VAL:HG22 | 1.93                     | 0.68              |
| 1:CA:511:C:C2     | 1:CA:512:U:C5      | 2.82                     | 0.68              |
| 22:DA:2297:A:C2   | 22:DA:2298:A:C8    | 2.81                     | 0.68              |
| 22:DA:2502:G:OP2  | 57:DA:3491:HOH:O   | 2.11                     | 0.68              |
| 1:AA:1093:A:N3    | 1:AA:1109:C:O2'    | 2.20                     | 0.68              |
| 53:B5:50:ILE:O    | 53:B5:203:GLU:CB   | 2.41                     | 0.68              |
| 22:DA:1469:A:C2   | 22:DA:1470:A:C6    | 2.81                     | 0.68              |
| 22:DA:1973:G:C6   | 22:DA:1974:C:C4    | 2.82                     | 0.68              |
| 22:DA:2199:A:C6   | 22:DA:2200:C:C2    | 2.81                     | 0.68              |
| 23:DB:84:G:N2     | 23:DB:93:C:C2      | 2.61                     | 0.68              |
| 24:DC:204:VAL:O   | 24:DC:206:GLY:N    | 2.27                     | 0.68              |
| 4:AD:59:GLN:O     | 4:AD:63:ARG:HG2    | 1.94                     | 0.68              |
| 25:BD:99:GLU:HG2  | 25:BD:182:ALA:HB2  | 1.73                     | 0.68              |
| 1:CA:475:C:H2'    | 1:CA:476:U:C6      | 2.28                     | 0.68              |
| 1:CA:620:C:C2     | 4:CD:132:ILE:HD13  | 2.29                     | 0.68              |
| 1:CA:801:U:C2     | 1:CA:802:A:C8      | 2.81                     | 0.68              |
| 35:DN:63:ARG:NH1  | 35:DN:81:ASN:OD1   | 2.26                     | 0.68              |
| 1:AA:1299:A:H2'   | 1:AA:1299:A:N3     | 2.09                     | 0.68              |
| 16:AP:60:TRP:O    | 16:AP:63:GLN:N     | 2.27                     | 0.68              |
| 12:CL:20:ASN:N    | 12:CL:20:ASN:OD1   | 2.26                     | 0.68              |
| 22:DA:2146:C:H5'' | 22:DA:2147:A:OP1   | 1.92                     | 0.68              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:DA:2788:C:O2'  | 22:DA:2809:A:N3   | 2.23                     | 0.68              |
| 22:DA:287:G:C2    | 22:DA:354:A:C2    | 2.82                     | 0.68              |
| 22:BA:2584:U:C5   | 22:BA:2585:U:C6   | 2.81                     | 0.68              |
| 22:BA:357:C:H2'   | 22:BA:358:U:C6    | 2.28                     | 0.68              |
| 22:DA:1351:C:OP2  | 57:DA:3397:HOH:O  | 2.11                     | 0.68              |
| 22:DA:2575:C:OP2  | 57:DA:3707:HOH:O  | 2.10                     | 0.68              |
| 22:DA:1638:C:H5'' | 22:DA:2710:C:O2'  | 1.93                     | 0.68              |
| 22:DA:590:A:C6    | 22:DA:591:U:C4    | 2.82                     | 0.68              |
| 30:DI:80:LEU:HD13 | 30:DI:136:MET:SD  | 2.33                     | 0.68              |
| 25:BD:62:LYS:HB2  | 25:BD:63:PRO:HD3  | 1.76                     | 0.68              |
| 1:CA:1408:A:C2    | 1:CA:1494:G:C4    | 2.82                     | 0.68              |
| 22:DA:1411:U:H2'  | 22:DA:1412:U:O4'  | 1.94                     | 0.68              |
| 22:DA:2453:A:N7   | 57:DA:3525:HOH:O  | 2.25                     | 0.68              |
| 22:DA:827:U:OP2   | 57:DA:3696:HOH:O  | 2.11                     | 0.68              |
| 35:DN:55:ALA:HA   | 35:DN:80:PHE:CE1  | 2.28                     | 0.68              |
| 1:AA:81:A:H2'     | 1:AA:82:G:H5''    | 1.76                     | 0.68              |
| 4:AD:3:ARG:CZ     | 4:AD:115:ARG:HD3  | 2.23                     | 0.68              |
| 22:BA:2032:G:N7   | 57:BA:3537:HOH:O  | 2.25                     | 0.68              |
| 22:BA:618:G:N7    | 57:BA:3287:HOH:O  | 2.27                     | 0.68              |
| 22:BA:792:A:N3    | 22:BA:2072:C:O2'  | 2.22                     | 0.68              |
| 22:DA:301:G:O4'   | 22:DA:317:G:N2    | 2.27                     | 0.68              |
| 22:DA:593:U:H2'   | 22:DA:594:U:C6    | 2.29                     | 0.68              |
| 22:DA:826:U:O2'   | 33:DL:53:GLY:HA3  | 1.94                     | 0.68              |
| 1:AA:1370:G:O5'   | 9:AI:111:VAL:HG21 | 1.94                     | 0.68              |
| 1:CA:227:G:H2'    | 1:CA:228:A:O4'    | 1.93                     | 0.68              |
| 27:DF:123:ASP:OD1 | 27:DF:124:GLY:N   | 2.27                     | 0.68              |
| 1:CA:1297:G:O2'   | 7:CG:114:LYS:NZ   | 2.21                     | 0.68              |
| 1:CA:1316:G:N1    | 1:CA:1319:A:OP2   | 2.27                     | 0.68              |
| 1:CA:706:A:C5     | 1:CA:707:U:C5     | 2.82                     | 0.68              |
| 22:DA:271:G:C2    | 22:DA:367:G:C2    | 2.82                     | 0.68              |
| 22:DA:425:G:C2    | 22:DA:426:C:C4    | 2.81                     | 0.68              |
| 19:AS:22:ALA:O    | 19:AS:26:GLY:N    | 2.27                     | 0.67              |
| 22:BA:1435:G:O2'  | 22:BA:1436:G:H5'  | 1.93                     | 0.67              |
| 22:BA:555:G:O2'   | 22:BA:556:A:OP2   | 2.11                     | 0.67              |
| 42:BU:82:ARG:O    | 42:BU:97:LYS:HG2  | 1.93                     | 0.67              |
| 1:CA:802:A:C2     | 1:CA:803:G:H1'    | 2.28                     | 0.67              |
| 4:CD:105:MET:SD   | 4:CD:143:VAL:HG13 | 2.33                     | 0.67              |
| 22:DA:1737:G:C6   | 22:DA:1738:G:N1   | 2.63                     | 0.67              |
| 22:DA:185:G:C6    | 22:DA:212:G:C2    | 2.82                     | 0.67              |
| 22:DA:2655:G:O2'  | 22:DA:2656:U:P    | 2.51                     | 0.67              |
| 25:BD:125:TRP:CD2 | 25:BD:160:LYS:HD2 | 2.29                     | 0.67              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 29:BH:122:LEU:HD23 | 29:BH:123:ARG:N    | 2.10                     | 0.67              |
| 1:CA:1490:U:H2'    | 1:CA:1491:G:O4'    | 1.93                     | 0.67              |
| 22:DA:1638:C:O2    | 22:DA:2698:U:O2'   | 2.11                     | 0.67              |
| 22:DA:2504:U:C5    | 55:DA:3001:DOL:C16 | 2.77                     | 0.67              |
| 25:DD:97:SER:O     | 25:DD:99:GLU:N     | 2.27                     | 0.67              |
| 32:DK:107:LEU:O    | 32:DK:109:SER:N    | 2.27                     | 0.67              |
| 22:BA:1421:G:C2    | 22:BA:1422:G:C8    | 2.83                     | 0.67              |
| 23:BB:116:G:H4'    | 36:BO:54:VAL:HG13  | 1.75                     | 0.67              |
| 33:BL:68:SER:O     | 33:BL:69:ARG:HB2   | 1.94                     | 0.67              |
| 22:DA:2874:C:H2'   | 22:DA:2875:C:C6    | 2.29                     | 0.67              |
| 25:BD:101:PHE:O    | 25:BD:103:ASP:N    | 2.26                     | 0.67              |
| 1:CA:1279:G:H2'    | 1:CA:1279:G:N3     | 2.08                     | 0.67              |
| 1:CA:499:A:C6      | 1:CA:547:A:C8      | 2.82                     | 0.67              |
| 1:CA:718:A:C5      | 11:CK:118:HIS:CD2  | 2.83                     | 0.67              |
| 9:CI:19:VAL:HG21   | 9:CI:82:GLY:HA3    | 1.77                     | 0.67              |
| 22:DA:2091:C:H3'   | 22:DA:2092:U:H5''  | 1.75                     | 0.67              |
| 22:DA:2111:U:C5    | 22:DA:2145:C:H2'   | 2.29                     | 0.67              |
| 14:AN:91:GLY:O     | 14:AN:93:ILE:N     | 2.27                     | 0.67              |
| 22:BA:1494:A:C2    | 22:BA:1495:A:C4    | 2.83                     | 0.67              |
| 12:CL:25:GLU:O     | 12:CL:27:CYS:N     | 2.27                     | 0.67              |
| 22:DA:2171:A:O2'   | 22:DA:2173:A:OP1   | 2.12                     | 0.67              |
| 23:DB:48:U:H4'     | 36:DO:100:HIS:CD2  | 2.30                     | 0.67              |
| 25:DD:140:HIS:NE2  | 57:DD:303:HOH:O    | 2.28                     | 0.67              |
| 22:BA:682:G:H5'    | 50:B2:26:ASN:OD1   | 1.95                     | 0.67              |
| 22:BA:2728:U:O2'   | 22:BA:2729:G:P     | 2.53                     | 0.67              |
| 1:CA:1151:A:C2     | 1:CA:1152:A:C5     | 2.82                     | 0.67              |
| 2:CB:96:TRP:CE2    | 2:CB:172:ALA:HB2   | 2.29                     | 0.67              |
| 2:CB:21:ARG:HA     | 2:CB:21:ARG:CZ     | 2.25                     | 0.67              |
| 4:CD:174:ASP:CG    | 4:CD:175:ALA:N     | 2.48                     | 0.67              |
| 5:CE:146:ASN:OD1   | 5:CE:146:ASN:N     | 2.27                     | 0.67              |
| 1:AA:1322:C:OP1    | 19:AS:78:ARG:NH2   | 2.28                     | 0.67              |
| 7:AG:13:LEU:O      | 7:AG:15:ASP:N      | 2.27                     | 0.67              |
| 22:BA:475:C:C4     | 22:BA:481:G:O6     | 2.48                     | 0.67              |
| 22:DA:1223:G:N2    | 22:DA:1226:A:OP2   | 2.24                     | 0.67              |
| 22:DA:1607:C:N4    | 22:DA:1622:G:N7    | 2.43                     | 0.67              |
| 22:DA:271:G:H4'    | 22:DA:272:A:OP1    | 1.94                     | 0.67              |
| 22:DA:453:A:OP1    | 57:DA:3242:HOH:O   | 2.12                     | 0.67              |
| 22:DA:846:U:O2'    | 22:DA:847:U:O5'    | 2.12                     | 0.67              |
| 1:AA:258:G:O6      | 57:AA:1811:HOH:O   | 2.12                     | 0.67              |
| 15:AO:63:ARG:HG2   | 15:AO:67:LEU:HD12  | 1.77                     | 0.67              |
| 22:BA:726:G:O2'    | 22:BA:727:A:OP2    | 2.13                     | 0.67              |

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| Atom-1            | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 26:BE:111:GLU:HG2 | 26:BE:114:ARG:NH1   | 2.10                     | 0.67              |
| 22:DA:2707:U:O2   | 35:DN:71:ARG:NH1    | 2.28                     | 0.67              |
| 22:DA:1138:G:O2'  | 31:DJ:104:ALA:O     | 2.12                     | 0.67              |
| 22:BA:1057:A:N6   | 22:BA:1087:G:OP2    | 2.28                     | 0.67              |
| 22:BA:1924:C:C2'  | 22:BA:1925:C:H5''   | 2.24                     | 0.67              |
| 22:BA:2346:A:H4'  | 22:BA:2347:C:OP2    | 1.93                     | 0.67              |
| 22:BA:826:U:O2'   | 33:BL:53:GLY:HA3    | 1.94                     | 0.67              |
| 30:BI:39:CYS:HA   | 30:BI:42:PHE:CB     | 2.25                     | 0.67              |
| 22:DA:247:G:H4'   | 22:DA:386:G:C4      | 2.30                     | 0.67              |
| 28:DG:118:PRO:CG  | 28:DG:144:VAL:HG21  | 2.25                     | 0.67              |
| 42:DU:38:GLY:HA2  | 42:DU:41:LEU:CD2    | 2.25                     | 0.67              |
| 8:AH:111:MET:HE1  | 8:AH:116:ALA:HA     | 1.77                     | 0.67              |
| 22:BA:2063:C:O2'  | 55:BA:3001:DOL:H343 | 1.95                     | 0.67              |
| 22:BA:2886:A:C5   | 22:BA:2887:A:C8     | 2.83                     | 0.67              |
| 29:BH:27:ARG:O    | 29:BH:28:ASN:HB2    | 1.95                     | 0.67              |
| 40:BS:83:LYS:O    | 40:BS:84:ARG:HD3    | 1.95                     | 0.67              |
| 1:CA:1381:U:C2'   | 1:CA:1382:C:O5'     | 2.43                     | 0.67              |
| 1:CA:919:A:C2     | 1:CA:920:U:C5       | 2.83                     | 0.67              |
| 2:CB:203:ASN:OD1  | 2:CB:204:ASP:N      | 2.27                     | 0.67              |
| 1:CA:427:U:OP1    | 4:CD:13:ARG:NH2     | 2.28                     | 0.67              |
| 30:DI:58:VAL:HG12 | 30:DI:59:ILE:N      | 2.10                     | 0.67              |
| 1:AA:209:U:H4'    | 1:AA:210:C:OP2      | 1.94                     | 0.66              |
| 22:BA:1922:G:N3   | 22:BA:1922:G:H2'    | 2.10                     | 0.66              |
| 22:BA:2499:C:OP2  | 57:BA:3687:HOH:O    | 2.13                     | 0.66              |
| 22:BA:1277:G:H5'  | 35:BN:20:MET:CE     | 2.25                     | 0.66              |
| 22:DA:577:G:O2'   | 22:DA:1254:A:OP1    | 2.13                     | 0.66              |
| 22:DA:912:C:N4    | 22:DA:913:U:O4      | 2.28                     | 0.66              |
| 22:DA:2603:G:C6   | 22:DA:2604:U:C4     | 2.83                     | 0.66              |
| 55:DA:3001:DOL:C1 | 55:DA:3001:DOL:C43  | 2.73                     | 0.66              |
| 32:DK:87:LEU:HD22 | 32:DK:92:GLU:HA     | 1.76                     | 0.66              |
| 14:AN:51:LEU:O    | 14:AN:53:ARG:N      | 2.28                     | 0.66              |
| 22:BA:1584:U:H2'  | 22:BA:1584:U:O2     | 1.95                     | 0.66              |
| 22:BA:1838:C:C5   | 22:BA:1899:A:C6     | 2.83                     | 0.66              |
| 29:BH:94:ILE:CG2  | 29:BH:99:ILE:HG13   | 2.26                     | 0.66              |
| 1:CA:309:A:O2'    | 1:CA:607:A:N1       | 2.27                     | 0.66              |
| 4:CD:105:MET:SD   | 4:CD:143:VAL:CG1    | 2.84                     | 0.66              |
| 18:CR:20:GLU:N    | 18:CR:55:LEU:HD12   | 2.09                     | 0.66              |
| 22:DA:2453:A:C2   | 57:DA:3529:HOH:O    | 2.48                     | 0.66              |
| 1:AA:1018:G:N3    | 1:AA:1018:G:H2'     | 2.11                     | 0.66              |
| 1:AA:582:C:C2     | 1:AA:583:A:C8       | 2.83                     | 0.66              |
| 39:BR:24:LYS:HA   | 39:BR:94:THR:HG23   | 1.77                     | 0.66              |

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| Atom-1            | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 1:CA:1345:U:C2    | 1:CA:1377:A:C2      | 2.84                     | 0.66              |
| 22:DA:1131:G:O6   | 22:DA:2024:G:O2'    | 2.13                     | 0.66              |
| 22:DA:1525:A:C2   | 22:DA:1526:C:C2     | 2.82                     | 0.66              |
| 22:DA:2594:C:N4   | 22:DA:2595:G:O6     | 2.28                     | 0.66              |
| 22:DA:2843:G:N2   | 22:DA:2875:C:C2     | 2.64                     | 0.66              |
| 42:DU:7:ARG:HG3   | 42:DU:8:ASP:N       | 2.11                     | 0.66              |
| 1:AA:1204:A:OP1   | 57:AA:1782:HOH:O    | 2.13                     | 0.66              |
| 1:AA:89:U:O2'     | 1:AA:90:C:C5'       | 2.44                     | 0.66              |
| 2:AB:181:ILE:O    | 2:AB:183:VAL:HG23   | 1.95                     | 0.66              |
| 22:BA:2325:G:C6   | 22:BA:2326:C:N4     | 2.63                     | 0.66              |
| 25:BD:133:THR:CG2 | 25:BD:134:HIS:CD2   | 2.78                     | 0.66              |
| 39:BR:66:HIS:ND1  | 39:BR:94:THR:HG22   | 2.10                     | 0.66              |
| 5:CE:56:VAL:N     | 5:CE:57:PRO:HD2     | 2.11                     | 0.66              |
| 22:DA:2056:G:O6   | 22:DA:2612:C:N3     | 2.28                     | 0.66              |
| 24:BC:15:HIS:O    | 24:BC:204:VAL:HG21  | 1.95                     | 0.66              |
| 27:BF:21:ASN:O    | 27:BF:21:ASN:ND2    | 2.28                     | 0.66              |
| 1:AA:1191:A:OP2   | 3:AC:3:GLN:NE2      | 2.29                     | 0.66              |
| 22:BA:1924:C:H2'  | 22:BA:1925:C:C5'    | 2.26                     | 0.66              |
| 22:BA:528:A:C2    | 22:BA:2043:C:H4'    | 2.30                     | 0.66              |
| 11:CK:27:PHE:CZ   | 11:CK:89:PRO:HG2    | 2.30                     | 0.66              |
| 22:DA:1509:A:O2'  | 22:DA:1510:G:OP2    | 2.14                     | 0.66              |
| 22:DA:2580:U:OP2  | 57:DA:3540:HOH:O    | 2.13                     | 0.66              |
| 22:DA:363:G:H2'   | 22:DA:364:C:C6      | 2.31                     | 0.66              |
| 22:DA:674:G:H1'   | 26:DE:69:ARG:NE     | 2.11                     | 0.66              |
| 20:AT:83:ILE:O    | 20:AT:87:ALA:HB3    | 1.95                     | 0.66              |
| 1:CA:1356:G:H2'   | 1:CA:1357:A:C8      | 2.30                     | 0.66              |
| 6:CF:45:ARG:O     | 6:CF:56:LYS:HA      | 1.96                     | 0.66              |
| 22:DA:1141:U:H4'  | 22:DA:1142:A:O4'    | 1.95                     | 0.66              |
| 22:DA:2452:C:C4'  | 55:DA:3001:DOL:H461 | 2.25                     | 0.66              |
| 26:DE:149:ILE:CD1 | 26:DE:172:ALA:HA    | 2.24                     | 0.66              |
| 1:AA:859:G:H2'    | 1:AA:860:A:C8       | 2.30                     | 0.66              |
| 15:AO:63:ARG:HG2  | 15:AO:67:LEU:CD1    | 2.26                     | 0.66              |
| 22:BA:2683:C:OP1  | 37:BP:51:ARG:NH2    | 2.28                     | 0.66              |
| 22:BA:817:C:OP1   | 57:BA:3583:HOH:O    | 2.12                     | 0.66              |
| 22:BA:933:A:H5'   | 22:BA:934:U:OP2     | 1.95                     | 0.66              |
| 24:BC:136:PRO:O   | 24:BC:139:SER:OG    | 2.09                     | 0.66              |
| 1:CA:1225:A:H2'   | 1:CA:1226:C:C5      | 2.29                     | 0.66              |
| 1:CA:70:U:H2'     | 1:CA:94:G:N7        | 2.11                     | 0.66              |
| 8:CH:2:SER:O      | 8:CH:4:GLN:N        | 2.29                     | 0.66              |
| 18:CR:22:ASP:OD1  | 18:CR:23:TYR:N      | 2.28                     | 0.66              |
| 22:DA:1454:C:OP1  | 35:DN:63:ARG:NH2    | 2.29                     | 0.66              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:DA:1475:G:O2'   | 22:DA:1476:U:P     | 2.53                     | 0.66              |
| 22:DA:226:A:N6     | 22:DA:227:A:N1     | 2.44                     | 0.66              |
| 22:DA:341:C:H2'    | 22:DA:342:A:C8     | 2.30                     | 0.66              |
| 22:DA:2838:G:O2'   | 35:DN:45:ARG:NH1   | 2.28                     | 0.66              |
| 1:AA:1493:A:OP2    | 1:AA:1493:A:C8     | 2.49                     | 0.66              |
| 30:BI:97:LYS:CG    | 30:BI:139:VAL:HG22 | 2.26                     | 0.66              |
| 35:BN:73:ASN:HA    | 35:BN:76:VAL:HG12  | 1.78                     | 0.66              |
| 4:CD:99:ASP:OD1    | 4:CD:100:ASN:N     | 2.29                     | 0.66              |
| 6:CF:8:PHE:CZ      | 6:CF:60:VAL:HB     | 2.31                     | 0.66              |
| 22:DA:1607:C:O2    | 22:DA:1621:U:C4    | 2.49                     | 0.66              |
| 30:DI:69:PHE:N     | 30:DI:69:PHE:CD1   | 2.64                     | 0.66              |
| 22:BA:2189:U:H2'   | 22:BA:2190:G:N9    | 2.10                     | 0.65              |
| 22:BA:2711:A:OP2   | 57:BA:3552:HOH:O   | 2.14                     | 0.65              |
| 22:BA:622:G:OP2    | 57:BA:3294:HOH:O   | 2.14                     | 0.65              |
| 41:BT:2:ILE:CA     | 41:BT:3:ARG:HB2    | 2.26                     | 0.65              |
| 1:CA:1391:U:H2'    | 1:CA:1392:G:C8     | 2.30                     | 0.65              |
| 1:CA:485:U:OP2     | 1:CA:485:U:H4'     | 1.96                     | 0.65              |
| 1:CA:604:G:H2'     | 1:CA:605:U:O4'     | 1.96                     | 0.65              |
| 5:CE:133:PRO:O     | 5:CE:137:VAL:HG12  | 1.95                     | 0.65              |
| 22:DA:104:A:N7     | 22:DA:105:C:C4     | 2.64                     | 0.65              |
| 22:DA:1623:G:C5    | 22:DA:1624:U:C5    | 2.84                     | 0.65              |
| 22:DA:2550:G:O6    | 22:DA:2551:C:N4    | 2.28                     | 0.65              |
| 1:AA:926:G:N2      | 1:AA:1505:G:H2'    | 2.12                     | 0.65              |
| 16:AP:10:GLY:HA3   | 16:AP:15:PRO:HA    | 1.78                     | 0.65              |
| 27:BF:132:VAL:HG22 | 27:BF:152:LEU:HB3  | 1.78                     | 0.65              |
| 2:CB:206:ALA:O     | 2:CB:208:ARG:N     | 2.29                     | 0.65              |
| 22:DA:1444:G:C2    | 22:DA:1548:A:C2    | 2.84                     | 0.65              |
| 48:B0:55:ILE:O     | 48:B0:56:ALA:CB    | 2.44                     | 0.65              |
| 22:BA:1509:A:HO2'  | 22:BA:1510:G:P     | 2.16                     | 0.65              |
| 29:BH:14:SER:O     | 29:BH:15:LEU:HB2   | 1.95                     | 0.65              |
| 32:BK:70:ARG:HD3   | 32:BK:76:VAL:HG22  | 1.78                     | 0.65              |
| 46:BY:35:GLY:O     | 46:BY:36:GLN:O     | 2.14                     | 0.65              |
| 1:CA:1105:A:C2     | 1:CA:1106:G:N7     | 2.65                     | 0.65              |
| 22:DA:2788:C:H2'   | 22:DA:2789:C:C6    | 2.31                     | 0.65              |
| 22:DA:618:G:N7     | 57:DA:3289:HOH:O   | 2.28                     | 0.65              |
| 32:DK:73:ASP:OD2   | 32:DK:75:SER:OG    | 2.14                     | 0.65              |
| 22:BA:1688:U:H1'   | 22:BA:1701:A:C6    | 2.32                     | 0.65              |
| 22:BA:447:A:OP2    | 57:BA:3210:HOH:O   | 2.14                     | 0.65              |
| 26:BE:108:ILE:HD11 | 26:BE:180:LEU:HB3  | 1.79                     | 0.65              |
| 42:BU:49:VAL:O     | 42:BU:49:VAL:CG2   | 2.44                     | 0.65              |
| 22:DA:1203:U:H1'   | 33:DL:4:ASN:HB3    | 1.79                     | 0.65              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 22:DA:2061:G:H2'   | 22:DA:2501:C:O2'  | 1.96                     | 0.65              |
| 22:DA:443:A:N7     | 26:DE:40:ARG:CG   | 2.59                     | 0.65              |
| 22:DA:564:C:O4'    | 38:DQ:37:GLN:NE2  | 2.29                     | 0.65              |
| 11:AK:13:ARG:N     | 22:BA:2141:G:H4'  | 2.11                     | 0.65              |
| 48:B0:33:THR:O     | 48:B0:33:THR:HG22 | 1.97                     | 0.65              |
| 22:BA:1439:A:C2    | 22:BA:1553:A:C5   | 2.85                     | 0.65              |
| 27:BF:2:ALA:O      | 27:BF:4:LEU:N     | 2.30                     | 0.65              |
| 29:BH:139:PHE:O    | 29:BH:140:ALA:CB  | 2.44                     | 0.65              |
| 30:BI:19:ASN:N     | 30:BI:20:PRO:CD   | 2.60                     | 0.65              |
| 1:CA:1127:G:H5'    | 1:CA:1280:A:O2'   | 1.96                     | 0.65              |
| 1:CA:378:G:C2      | 1:CA:386:C:O2     | 2.50                     | 0.65              |
| 1:CA:858:G:O6      | 1:CA:869:G:H3'    | 1.96                     | 0.65              |
| 22:DA:192:C:N4     | 22:DA:193:U:O2    | 2.29                     | 0.65              |
| 26:DE:108:ILE:HD13 | 26:DE:181:ILE:CG1 | 2.26                     | 0.65              |
| 7:AG:111:ARG:NH1   | 7:AG:123:GLU:OE2  | 2.29                     | 0.65              |
| 11:AK:34:ILE:HB    | 11:AK:74:VAL:HG11 | 1.77                     | 0.65              |
| 17:AQ:12:VAL:HG12  | 17:AQ:13:VAL:N    | 2.10                     | 0.65              |
| 17:AQ:53:CYS:SG    | 17:AQ:75:LEU:HD23 | 2.37                     | 0.65              |
| 22:BA:2043:C:OP1   | 22:BA:2777:G:O2'  | 2.12                     | 0.65              |
| 22:BA:636:G:N7     | 33:BL:109:LYS:NZ  | 2.39                     | 0.65              |
| 25:BD:104:VAL:O    | 25:BD:105:LYS:HB2 | 1.97                     | 0.65              |
| 29:BH:114:GLU:HB3  | 29:BH:133:GLN:O   | 1.97                     | 0.65              |
| 1:CA:160:A:H2'     | 1:CA:161:A:O4'    | 1.97                     | 0.65              |
| 22:DA:2164:C:H2'   | 22:DA:2165:C:C6   | 2.32                     | 0.65              |
| 22:DA:2226:C:H2'   | 22:DA:2227:A:O4'  | 1.97                     | 0.65              |
| 22:DA:2306:C:OP2   | 22:DA:2307:G:O2'  | 2.07                     | 0.65              |
| 22:DA:2467:C:N4    | 22:DA:2468:A:C6   | 2.65                     | 0.65              |
| 22:DA:277:G:H3'    | 22:DA:277:G:N3    | 2.11                     | 0.65              |
| 22:DA:35:G:C4      | 22:DA:454:A:C2    | 2.84                     | 0.65              |
| 22:DA:866:A:O4'    | 22:DA:914:G:N2    | 2.30                     | 0.65              |
| 46:DY:56:LEU:O     | 46:DY:57:LEU:CB   | 2.45                     | 0.65              |
| 1:AA:1320:C:N3     | 19:AS:36:ARG:NH1  | 2.43                     | 0.65              |
| 1:AA:89:U:O2'      | 1:AA:90:C:H5"     | 1.96                     | 0.65              |
| 5:AE:90:THR:HG22   | 5:AE:91:GLY:N     | 2.11                     | 0.65              |
| 48:B0:48:TYR:CE2   | 48:B0:53:LYS:HB2  | 2.32                     | 0.65              |
| 22:BA:2063:C:O2    | 22:BA:2450:A:N1   | 2.29                     | 0.65              |
| 22:BA:2269:G:OP1   | 57:BA:3513:HOH:O  | 2.14                     | 0.65              |
| 1:CA:1460:C:N4     | 1:CA:1461:G:C6    | 2.65                     | 0.65              |
| 1:CA:801:U:H2'     | 1:CA:802:A:H8     | 1.62                     | 0.65              |
| 22:DA:2079:U:H2'   | 22:DA:2080:A:O4'  | 1.96                     | 0.65              |
| 22:DA:70:G:N2      | 22:DA:71:A:N1     | 2.44                     | 0.65              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:DA:2599:G:N7   | 24:DC:236:GLU:HB3  | 2.12                     | 0.65              |
| 35:DN:107:ASN:O   | 35:DN:107:ASN:ND2  | 2.30                     | 0.65              |
| 1:AA:657:U:O2     | 15:AO:22:THR:CG2   | 2.45                     | 0.65              |
| 22:BA:747:U:C4    | 22:BA:2613:U:C5    | 2.84                     | 0.65              |
| 22:BA:2800:A:C2   | 22:BA:2895:G:H1'   | 2.31                     | 0.65              |
| 11:CK:88:GLY:N    | 11:CK:114:THR:HG22 | 2.11                     | 0.65              |
| 22:DA:996:A:C2    | 22:DA:997:G:C8     | 2.85                     | 0.65              |
| 34:DM:19:GLY:O    | 34:DM:38:ARG:NH1   | 2.29                     | 0.65              |
| 22:BA:1358:G:N7   | 57:BA:3406:HOH:O   | 2.30                     | 0.65              |
| 22:BA:813:U:H2'   | 22:BA:814:C:C6     | 2.32                     | 0.65              |
| 39:BR:39:LEU:HA   | 39:BR:49:ILE:HG23  | 1.79                     | 0.65              |
| 1:CA:17:U:H2'     | 1:CA:18:C:C6       | 2.31                     | 0.65              |
| 1:CA:485:U:O2'    | 1:CA:486:U:OP1     | 2.14                     | 0.65              |
| 22:DA:1359:A:C8   | 22:DA:1373:A:N1    | 2.65                     | 0.65              |
| 22:DA:2589:A:OP1  | 57:DA:3311:HOH:O   | 2.14                     | 0.65              |
| 22:DA:301:G:H1'   | 22:DA:302:C:C6     | 2.32                     | 0.65              |
| 22:DA:757:G:N7    | 57:DA:3303:HOH:O   | 2.29                     | 0.65              |
| 1:AA:597:G:C2     | 1:AA:644:U:C2      | 2.84                     | 0.65              |
| 12:AL:21:VAL:HG23 | 12:AL:95:TYR:CE1   | 2.31                     | 0.65              |
| 14:AN:54:ASP:OD1  | 14:AN:59:ARG:NH1   | 2.27                     | 0.65              |
| 53:B5:121:MET:CB  | 53:B5:143:ALA:HB1  | 2.27                     | 0.65              |
| 22:BA:1078:U:H1'  | 22:BA:1088:A:C2    | 2.32                     | 0.65              |
| 22:BA:2711:A:P    | 57:BA:3550:HOH:O   | 2.55                     | 0.65              |
| 22:BA:858:G:H3'   | 22:BA:859:G:C8     | 2.32                     | 0.65              |
| 1:CA:154:U:C2     | 1:CA:168:G:N2      | 2.65                     | 0.65              |
| 1:CA:64:G:C8      | 1:CA:99:C:N4       | 2.65                     | 0.65              |
| 4:CD:174:ASP:O    | 4:CD:175:ALA:CB    | 2.44                     | 0.65              |
| 19:CS:66:MET:SD   | 19:CS:74:PHE:CZ    | 2.90                     | 0.65              |
| 22:DA:1237:A:H4'  | 22:DA:1238:G:OP1   | 1.96                     | 0.65              |
| 1:AA:1062:U:H2'   | 1:AA:1063:C:C6     | 2.32                     | 0.64              |
| 5:AE:82:GLN:HG2   | 5:AE:150:PRO:HB3   | 1.78                     | 0.64              |
| 7:AG:40:GLU:HB2   | 7:AG:44:TYR:CE2    | 2.32                     | 0.64              |
| 16:AP:79:ASN:O    | 16:AP:80:LYS:HB2   | 1.96                     | 0.64              |
| 22:BA:2637:U:C2'  | 22:BA:2638:G:H5'   | 2.27                     | 0.64              |
| 1:CA:8:A:C5       | 4:CD:206:LYS:HB3   | 2.31                     | 0.64              |
| 50:D2:35:ARG:O    | 50:D2:38:GLY:N     | 2.30                     | 0.64              |
| 22:DA:2307:G:OP1  | 22:DA:2308:G:N2    | 2.29                     | 0.64              |
| 22:DA:290:U:C4    | 22:DA:291:G:N7     | 2.65                     | 0.64              |
| 22:DA:54:G:C2     | 22:DA:55:G:C8      | 2.85                     | 0.64              |
| 22:DA:1566:A:C2   | 24:DC:213:TRP:CD2  | 2.85                     | 0.64              |
| 34:DM:2:LEU:O     | 34:DM:3:GLN:HB3    | 1.96                     | 0.64              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 35:DN:71:ARG:CG    | 35:DN:71:ARG:HH21  | 2.10                     | 0.64              |
| 1:AA:11:G:C5       | 1:AA:12:U:C5       | 2.85                     | 0.64              |
| 4:AD:130:VAL:HG11  | 4:AD:135:TYR:CD1   | 2.33                     | 0.64              |
| 8:AH:10:MET:HE1    | 8:AH:33:LYS:HB3    | 1.79                     | 0.64              |
| 51:B3:27:ALA:O     | 51:B3:28:ASN:HB2   | 1.98                     | 0.64              |
| 22:BA:1428:C:C5    | 22:BA:1569:A:H5''  | 2.32                     | 0.64              |
| 22:BA:733:G:OP2    | 57:BA:3296:HOH:O   | 2.14                     | 0.64              |
| 29:BH:122:LEU:C    | 29:BH:123:ARG:HG2  | 2.17                     | 0.64              |
| 4:CD:59:GLN:OE1    | 4:CD:59:GLN:HA     | 1.96                     | 0.64              |
| 16:CP:39:PHE:CD1   | 16:CP:74:LEU:HD11  | 2.32                     | 0.64              |
| 1:AA:1006:G:OP1    | 1:AA:1037:C:O2'    | 2.15                     | 0.64              |
| 1:AA:1053:G:O5'    | 1:AA:1054:C:H3'    | 1.96                     | 0.64              |
| 17:AQ:12:VAL:O     | 17:AQ:13:VAL:HG12  | 1.97                     | 0.64              |
| 22:BA:1700:A:H5'   | 22:BA:1701:A:OP2   | 1.97                     | 0.64              |
| 23:BB:30:C:H2'     | 23:BB:31:C:H5'     | 1.79                     | 0.64              |
| 28:BG:121:ILE:HD12 | 28:BG:141:ILE:HG22 | 1.78                     | 0.64              |
| 35:BN:33:ILE:HG13  | 35:BN:114:GLU:HB3  | 1.79                     | 0.64              |
| 1:CA:1007:U:H2'    | 1:CA:1008:U:C5'    | 2.27                     | 0.64              |
| 12:CL:57:LEU:O     | 12:CL:59:ASN:N     | 2.29                     | 0.64              |
| 22:DA:1416:G:C4    | 22:DA:1417:C:C5    | 2.86                     | 0.64              |
| 22:DA:1603:A:OP1   | 57:DA:3409:HOH:O   | 2.14                     | 0.64              |
| 22:DA:1802:A:C2    | 22:DA:1803:A:C4    | 2.85                     | 0.64              |
| 22:DA:2199:A:C5    | 22:DA:2225:A:C6    | 2.85                     | 0.64              |
| 22:DA:2824:C:N4    | 22:DA:2825:G:N7    | 2.45                     | 0.64              |
| 22:DA:694:U:C2'    | 22:DA:695:G:H5''   | 2.27                     | 0.64              |
| 22:DA:878:A:N6     | 22:DA:899:A:O2'    | 2.31                     | 0.64              |
| 1:AA:683:G:N2      | 11:AK:39:GLY:O     | 2.30                     | 0.64              |
| 17:AQ:16:LYS:N     | 17:AQ:17:MET:SD    | 2.71                     | 0.64              |
| 22:BA:747:U:C4     | 22:BA:2613:U:C4    | 2.86                     | 0.64              |
| 22:BA:2591:C:OP1   | 24:BC:238:ARG:NH1  | 2.29                     | 0.64              |
| 27:BF:176:PRO:O    | 27:BF:177:PHE:CG   | 2.51                     | 0.64              |
| 1:CA:1211:U:O2'    | 1:CA:1212:U:OP2    | 2.15                     | 0.64              |
| 1:CA:1255:G:C6     | 1:CA:1279:G:C8     | 2.86                     | 0.64              |
| 1:CA:945:G:C2      | 1:CA:946:A:C8      | 2.85                     | 0.64              |
| 2:CB:35:ARG:O      | 2:CB:37:LYS:N      | 2.31                     | 0.64              |
| 10:CJ:91:ASP:N     | 10:CJ:91:ASP:OD1   | 2.30                     | 0.64              |
| 22:DA:1438:U:C5    | 22:DA:1552:A:C2    | 2.86                     | 0.64              |
| 22:DA:1440:U:O4    | 57:DA:3628:HOH:O   | 2.14                     | 0.64              |
| 22:DA:72:U:O2'     | 22:DA:73:A:O5'     | 2.14                     | 0.64              |
| 1:AA:1310:G:OP2    | 13:AM:87:ARG:NH2   | 2.31                     | 0.64              |
| 5:AE:81:LEU:HB3    | 5:AE:147:MET:HE3   | 1.79                     | 0.64              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:AN:21:PHE:HA   | 14:AN:25:ALA:HB3  | 1.78                     | 0.64              |
| 22:BA:1153:C:P    | 57:BA:3364:HOH:O  | 2.54                     | 0.64              |
| 22:BA:1474:U:C2'  | 22:BA:1475:G:H5'  | 2.27                     | 0.64              |
| 24:BC:252:THR:O   | 24:BC:253:LYS:C   | 2.33                     | 0.64              |
| 26:BE:155:GLU:HA  | 26:BE:155:GLU:OE1 | 1.97                     | 0.64              |
| 39:BR:68:ARG:HD3  | 39:BR:92:TRP:CZ2  | 2.33                     | 0.64              |
| 2:CB:119:THR:O    | 2:CB:120:GLN:HB2  | 1.98                     | 0.64              |
| 9:CI:33:ARG:NE    | 9:CI:37:GLN:OE1   | 2.30                     | 0.64              |
| 22:DA:2147:A:H2'  | 22:DA:2148:G:O4'  | 1.98                     | 0.64              |
| 25:DD:12:THR:OG1  | 25:DD:13:ARG:N    | 2.30                     | 0.64              |
| 31:DJ:41:LYS:NZ   | 31:DJ:52:ASP:OD2  | 2.19                     | 0.64              |
| 33:DL:38:GLN:O    | 33:DL:40:SER:N    | 2.29                     | 0.64              |
| 37:DP:103:ARG:HB3 | 37:DP:108:ALA:HB2 | 1.80                     | 0.64              |
| 13:AM:114:LYS:CB  | 13:AM:115:PRO:HD3 | 2.26                     | 0.64              |
| 48:B0:15:MET:O    | 48:B0:18:SER:HB3  | 1.98                     | 0.64              |
| 1:CA:1061:G:O4'   | 10:CJ:58:ASN:ND2  | 2.31                     | 0.64              |
| 19:CS:55:ARG:NE   | 19:CS:79:THR:HG22 | 2.13                     | 0.64              |
| 22:DA:1027:A:C6   | 22:DA:1126:A:N3   | 2.66                     | 0.64              |
| 22:DA:583:G:C5    | 22:DA:584:C:C5    | 2.86                     | 0.64              |
| 10:AJ:35:GLN:CG   | 10:AJ:77:VAL:HB   | 2.27                     | 0.64              |
| 48:B0:55:ILE:O    | 48:B0:56:ALA:HB3  | 1.98                     | 0.64              |
| 22:BA:1869:G:H3'  | 22:BA:1870:C:H5'  | 1.80                     | 0.64              |
| 22:BA:2128:G:H2'  | 22:BA:2129:C:O4'  | 1.97                     | 0.64              |
| 35:BN:66:ALA:O    | 35:BN:69:ARG:O    | 2.15                     | 0.64              |
| 23:BB:116:G:H4'   | 36:BO:54:VAL:O    | 1.97                     | 0.64              |
| 1:CA:829:G:C5     | 1:CA:858:G:N2     | 2.66                     | 0.64              |
| 5:CE:65:GLU:OE1   | 5:CE:69:ARG:NH2   | 2.31                     | 0.64              |
| 9:CI:120:LYS:HG3  | 9:CI:123:ARG:HB3  | 1.78                     | 0.64              |
| 22:DA:1907:G:C2   | 22:DA:1924:C:C2   | 2.85                     | 0.64              |
| 1:AA:1500:A:OP2   | 57:AA:1872:HOH:O  | 2.14                     | 0.64              |
| 1:AA:49:U:O4      | 1:AA:365:U:H5     | 1.81                     | 0.64              |
| 1:AA:663:A:C2     | 1:AA:743:A:C2     | 2.86                     | 0.64              |
| 22:BA:2419:U:O2'  | 22:BA:2420:C:H5'  | 1.97                     | 0.64              |
| 1:CA:563:A:H2'    | 1:CA:567:G:C8     | 2.33                     | 0.64              |
| 1:CA:706:A:O2'    | 11:CK:31:ILE:HD11 | 1.98                     | 0.64              |
| 22:DA:144:A:C2    | 22:DA:145:C:C2    | 2.85                     | 0.64              |
| 22:DA:388:G:N7    | 22:DA:390:U:H2'   | 2.12                     | 0.64              |
| 22:DA:668:A:C2    | 22:DA:670:A:C5    | 2.86                     | 0.64              |
| 1:AA:650:G:C2'    | 1:AA:651:C:H5'    | 2.28                     | 0.64              |
| 3:AC:139:GLN:O    | 3:AC:141:ALA:N    | 2.29                     | 0.64              |
| 22:BA:1246:A:H2'  | 22:BA:1247:A:O5'  | 1.98                     | 0.64              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:BA:2343:U:HO2' | 22:BA:2373:G:HO2'  | 1.43                     | 0.64              |
| 22:BA:645:C:O2'   | 22:BA:646:U:H5''   | 1.98                     | 0.64              |
| 42:BU:12:ILE:CG2  | 42:BU:80:ALA:HB2   | 2.28                     | 0.64              |
| 1:CA:527:G:C6     | 1:CA:528:C:C5      | 2.86                     | 0.64              |
| 22:DA:192:C:C5    | 22:DA:193:U:C2     | 2.86                     | 0.64              |
| 22:DA:422:A:C2    | 22:DA:423:A:C4     | 2.86                     | 0.64              |
| 25:DD:208:LYS:O   | 25:DD:209:ALA:CB   | 2.46                     | 0.64              |
| 40:DS:66:ILE:O    | 40:DS:68:ASP:N     | 2.31                     | 0.64              |
| 4:AD:32:CYS:O     | 4:AD:33:LYS:HB2    | 1.98                     | 0.64              |
| 20:AT:81:ALA:O    | 20:AT:85:LYS:HG2   | 1.96                     | 0.64              |
| 22:BA:1916:A:H2'  | 22:BA:1917:U:H1'   | 1.80                     | 0.64              |
| 22:BA:2430:A:H5'  | 22:BA:2431:U:OP2   | 1.98                     | 0.64              |
| 22:BA:265:A:H4'   | 22:BA:266:G:OP1    | 1.98                     | 0.64              |
| 40:BS:73:LYS:HB2  | 40:BS:106:VAL:HB   | 1.79                     | 0.64              |
| 1:AA:841:C:O2'    | 2:CB:153:ASP:OD1   | 2.16                     | 0.64              |
| 17:CQ:21:ILE:N    | 17:CQ:48:ASP:OD1   | 2.30                     | 0.64              |
| 22:DA:1359:A:C8   | 22:DA:1373:A:C2    | 2.86                     | 0.64              |
| 22:DA:187:G:C2    | 22:DA:210:C:C2     | 2.86                     | 0.64              |
| 26:DE:128:ALA:O   | 26:DE:130:LYS:N    | 2.31                     | 0.64              |
| 34:DM:136:MET:O   | 43:DV:79:ARG:NH2   | 2.31                     | 0.64              |
| 22:BA:1009:A:OP1  | 31:BJ:39:LYS:NZ    | 2.31                     | 0.63              |
| 22:BA:2048:G:O6   | 57:BA:3680:HOH:O   | 2.11                     | 0.63              |
| 24:BC:8:PRO:HB3   | 24:BC:14:ARG:HB2   | 1.80                     | 0.63              |
| 1:CA:664:G:N2     | 1:CA:666:G:C8      | 2.66                     | 0.63              |
| 15:CO:18:ASP:OD1  | 15:CO:20:ASN:N     | 2.30                     | 0.63              |
| 22:DA:1440:U:O4   | 57:DA:3627:HOH:O   | 2.13                     | 0.63              |
| 22:DA:1676:A:H2'  | 22:DA:1677:A:O4'   | 1.99                     | 0.63              |
| 22:DA:2004:G:P    | 57:DA:3798:HOH:O   | 2.56                     | 0.63              |
| 22:DA:200:U:O4    | 22:DA:248:G:C2     | 2.51                     | 0.63              |
| 1:AA:663:A:N1     | 1:AA:743:A:C2      | 2.66                     | 0.63              |
| 53:B5:65:LEU:HD11 | 53:B5:191:ARG:CB   | 2.28                     | 0.63              |
| 22:BA:2820:A:N1   | 25:BD:197:THR:HG22 | 2.13                     | 0.63              |
| 38:BQ:79:PHE:CZ   | 38:BQ:83:LEU:HD11  | 2.34                     | 0.63              |
| 43:BV:80:HIS:CE1  | 43:BV:83:LYS:CG    | 2.81                     | 0.63              |
| 44:BW:37:ILE:HG21 | 44:BW:80:ILE:HG21  | 1.79                     | 0.63              |
| 8:CH:2:SER:C      | 8:CH:4:GLN:H       | 2.01                     | 0.63              |
| 22:DA:1097:U:C5   | 22:DA:1098:A:H1'   | 2.33                     | 0.63              |
| 22:DA:1668:A:O4'  | 22:DA:1669:A:C2    | 2.51                     | 0.63              |
| 22:DA:297:G:C8    | 57:DA:3229:HOH:O   | 2.49                     | 0.63              |
| 22:DA:352:A:H2'   | 22:DA:353:C:O4'    | 1.99                     | 0.63              |
| 29:DH:117:LEU:CD1 | 29:DH:130:VAL:HG22 | 2.28                     | 0.63              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:AB:123:ASP:OD1   | 2:AB:123:ASP:N     | 2.30                     | 0.63              |
| 22:BA:545:U:H3'    | 22:BA:546:U:H4'    | 1.80                     | 0.63              |
| 22:BA:996:A:C2     | 22:BA:997:G:C8     | 2.85                     | 0.63              |
| 24:BC:144:VAL:HG21 | 24:BC:162:VAL:HG21 | 1.79                     | 0.63              |
| 37:BP:53:ARG:CG    | 37:BP:53:ARG:HH11  | 2.11                     | 0.63              |
| 41:BT:1:MET:O      | 41:BT:2:ILE:HG13   | 1.97                     | 0.63              |
| 22:BA:58:G:OP1     | 41:BT:78:SER:HB2   | 1.98                     | 0.63              |
| 16:CP:14:ARG:N     | 16:CP:15:PRO:CD    | 2.61                     | 0.63              |
| 21:CU:21:ARG:HD3   | 21:CU:21:ARG:N     | 2.12                     | 0.63              |
| 22:DA:1363:C:O2    | 22:DA:1369:G:C2    | 2.51                     | 0.63              |
| 22:DA:276:U:H2'    | 22:DA:276:U:O2     | 1.98                     | 0.63              |
| 22:DA:668:A:N6     | 22:DA:670:A:O2'    | 2.32                     | 0.63              |
| 22:DA:727:A:H2'    | 22:DA:728:G:C8     | 2.34                     | 0.63              |
| 39:DR:38:VAL:HG11  | 39:DR:57:GLY:HA3   | 1.79                     | 0.63              |
| 11:AK:16:VAL:O     | 11:AK:17:SER:CB    | 2.46                     | 0.63              |
| 53:B5:87:ALA:HB2   | 53:B5:153:ILE:CB   | 2.28                     | 0.63              |
| 22:BA:322:A:C5     | 22:BA:340:A:C2     | 2.86                     | 0.63              |
| 39:BR:49:ILE:HB    | 39:BR:51:VAL:O     | 1.99                     | 0.63              |
| 1:CA:1167:A:N7     | 1:CA:1169:A:C5     | 2.67                     | 0.63              |
| 1:CA:404:G:N7      | 4:CD:2:ALA:N       | 2.46                     | 0.63              |
| 4:CD:34:ILE:O      | 4:CD:35:GLU:HB3    | 1.98                     | 0.63              |
| 15:CO:17:ARG:O     | 15:CO:18:ASP:CB    | 2.46                     | 0.63              |
| 22:DA:1096:A:H2'   | 22:DA:1097:U:O4'   | 1.97                     | 0.63              |
| 22:DA:2048:G:OP1   | 57:DA:3380:HOH:O   | 2.15                     | 0.63              |
| 22:DA:2408:U:O4    | 57:DA:3559:HOH:O   | 2.12                     | 0.63              |
| 22:DA:2636:C:H2'   | 22:DA:2637:U:C6    | 2.34                     | 0.63              |
| 22:DA:682:G:N2     | 22:DA:683:U:C2     | 2.66                     | 0.63              |
| 25:DD:149:ASN:OD1  | 25:DD:150:GLN:N    | 2.31                     | 0.63              |
| 29:DH:117:LEU:HG   | 29:DH:120:GLY:O    | 1.98                     | 0.63              |
| 35:DN:87:PHE:O     | 35:DN:90:ARG:N     | 2.32                     | 0.63              |
| 1:AA:373:A:C2      | 1:AA:374:A:C8      | 2.86                     | 0.63              |
| 1:AA:77:A:N1       | 1:AA:91:U:O4       | 2.30                     | 0.63              |
| 22:BA:1087:G:N2    | 22:BA:1090:A:C8    | 2.67                     | 0.63              |
| 22:BA:1768:C:C4    | 22:BA:1769:U:C5    | 2.87                     | 0.63              |
| 22:BA:572:A:OP2    | 39:BR:80:ARG:NH2   | 2.29                     | 0.63              |
| 40:BS:38:TYR:CD2   | 48:B0:39:LEU:HD21  | 2.33                     | 0.63              |
| 1:CA:1150:A:N6     | 1:CA:1151:A:H62    | 1.96                     | 0.63              |
| 3:CC:139:GLN:O     | 3:CC:141:ALA:N     | 2.31                     | 0.63              |
| 22:DA:1094:U:H2'   | 22:DA:1096:A:OP2   | 1.99                     | 0.63              |
| 22:DA:1805:A:C2    | 22:DA:1813:G:C2    | 2.86                     | 0.63              |
| 22:DA:945:A:C8     | 22:DA:2448:A:C2    | 2.86                     | 0.63              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 22:DA:2563:U:O4'   | 22:DA:2566:A:N6   | 2.31                     | 0.63              |
| 2:AB:219:ALA:O     | 2:AB:220:THR:HB   | 1.98                     | 0.63              |
| 4:AD:120:HIS:O     | 4:AD:121:LYS:C    | 2.37                     | 0.63              |
| 5:AE:65:GLU:OE1    | 5:AE:66:LYS:N     | 2.32                     | 0.63              |
| 22:BA:1317:G:C2    | 22:BA:1336:A:C2   | 2.86                     | 0.63              |
| 28:BG:80:THR:HG22  | 28:BG:81:GLU:N    | 2.12                     | 0.63              |
| 36:BO:31:THR:HG22  | 36:BO:34:HIS:H    | 1.64                     | 0.63              |
| 1:CA:1141:C:O2'    | 1:CA:1142:G:O5'   | 2.15                     | 0.63              |
| 13:CM:98:ARG:O     | 13:CM:100:GLN:N   | 2.31                     | 0.63              |
| 22:DA:1627:G:C2    | 22:DA:1628:G:C8   | 2.86                     | 0.63              |
| 22:DA:53:A:C8      | 22:DA:54:G:C8     | 2.87                     | 0.63              |
| 23:DB:44:G:N2      | 23:DB:48:U:O2     | 2.32                     | 0.63              |
| 33:DL:93:ASN:OD1   | 33:DL:94:THR:N    | 2.31                     | 0.63              |
| 1:AA:1161:C:H2'    | 1:AA:1162:C:C6    | 2.34                     | 0.63              |
| 22:BA:1746:A:H2'   | 22:BA:1747:U:H6   | 1.62                     | 0.63              |
| 22:BA:1917:U:C4    | 22:BA:1918:A:C5   | 2.87                     | 0.63              |
| 22:BA:1939:U:OP1   | 22:BA:2604:U:O2'  | 2.17                     | 0.63              |
| 11:CK:125:LYS:O    | 21:CU:34:ARG:NE   | 2.32                     | 0.63              |
| 22:DA:2652:C:C4    | 22:DA:2653:U:C4   | 2.86                     | 0.63              |
| 24:DC:33:LEU:O     | 24:DC:64:ILE:HD12 | 1.99                     | 0.63              |
| 25:DD:104:VAL:O    | 25:DD:105:LYS:CB  | 2.46                     | 0.63              |
| 1:AA:1181:G:O2'    | 1:AA:1182:G:C5    | 2.51                     | 0.63              |
| 23:BB:33:G:O2'     | 23:BB:34:A:H5'    | 1.99                     | 0.63              |
| 24:BC:237:GLY:C    | 57:BC:407:HOH:O   | 2.36                     | 0.63              |
| 25:BD:151:THR:HG22 | 25:BD:152:PRO:CD  | 2.29                     | 0.63              |
| 30:BI:39:CYS:HA    | 30:BI:42:PHE:HB3  | 1.80                     | 0.63              |
| 1:CA:1521:C:N3     | 1:CA:1522:U:C5    | 2.67                     | 0.63              |
| 22:DA:980:A:C4     | 22:DA:1136:G:O4'  | 2.51                     | 0.63              |
| 22:DA:1258:U:H2'   | 22:DA:1259:G:C8   | 2.33                     | 0.63              |
| 22:DA:1313:U:H4'   | 22:DA:1332:G:H4'  | 1.79                     | 0.63              |
| 22:DA:1390:U:H2'   | 22:DA:1391:U:H5'  | 1.81                     | 0.63              |
| 22:DA:1447:C:H2'   | 22:DA:1448:G:C8   | 2.34                     | 0.63              |
| 22:DA:1805:A:N3    | 22:DA:1813:G:C2   | 2.67                     | 0.63              |
| 22:DA:333:G:C5     | 22:DA:334:C:C5    | 2.87                     | 0.63              |
| 31:DJ:41:LYS:O     | 31:DJ:44:TYR:N    | 2.32                     | 0.63              |
| 22:BA:1695:G:H1'   | 24:BC:8:PRO:O     | 1.98                     | 0.63              |
| 22:BA:1717:A:C2'   | 22:BA:1718:G:O5'  | 2.47                     | 0.63              |
| 22:BA:1917:U:C2'   | 22:BA:1918:A:H5'  | 2.28                     | 0.63              |
| 26:BE:145:ASP:HB3  | 26:BE:184:ASP:OD2 | 1.99                     | 0.63              |
| 37:BP:64:ILE:O     | 37:BP:64:ILE:HG22 | 1.97                     | 0.63              |
| 12:CL:47:SER:O     | 12:CL:48:ALA:CB   | 2.47                     | 0.63              |

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| Atom-1           | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|---------------------|--------------------------|-------------------|
| 22:DA:2121:G:N2  | 22:DA:2177:C:O2     | 2.31                     | 0.63              |
| 1:AA:71:A:O2'    | 1:AA:72:A:OP2       | 2.16                     | 0.62              |
| 1:AA:807:A:C5    | 1:AA:808:C:C5       | 2.86                     | 0.62              |
| 14:AN:72:GLY:O   | 14:AN:80:SER:HA     | 1.99                     | 0.62              |
| 22:BA:2448:A:P   | 57:BA:3687:HOH:O    | 2.57                     | 0.62              |
| 22:BA:64:A:H2'   | 22:BA:65:U:C6       | 2.33                     | 0.62              |
| 1:CA:183:C:O2'   | 1:CA:184:G:O5'      | 2.16                     | 0.62              |
| 6:CF:32:ALA:O    | 6:CF:34:GLY:N       | 2.32                     | 0.62              |
| 24:DC:237:GLY:O  | 24:DC:239:ASN:N     | 2.32                     | 0.62              |
| 1:AA:1160:G:O6   | 1:AA:1181:G:C6      | 2.51                     | 0.62              |
| 1:AA:381:C:H2'   | 1:AA:382:A:O4'      | 1.97                     | 0.62              |
| 2:AB:73:LYS:O    | 2:AB:75:ALA:N       | 2.30                     | 0.62              |
| 11:AK:69:ARG:HD3 | 22:BA:2146:C:N3     | 2.14                     | 0.62              |
| 22:BA:731:C:P    | 57:BA:3695:HOH:O    | 2.52                     | 0.62              |
| 41:BT:33:LYS:HG3 | 41:BT:80:TRP:CE3    | 2.34                     | 0.62              |
| 1:CA:495:A:N1    | 1:CA:496:A:N6       | 2.46                     | 0.62              |
| 1:CA:815:A:N7    | 1:CA:1509:C:O2'     | 2.25                     | 0.62              |
| 22:DA:1707:G:N2  | 22:DA:1752:C:C2     | 2.67                     | 0.62              |
| 22:DA:2339:C:H2' | 22:DA:2340:A:C8     | 2.34                     | 0.62              |
| 22:DA:197:A:H62  | 22:DA:2430:A:H2'    | 1.64                     | 0.62              |
| 22:DA:2531:A:H5' | 28:DG:157:TYR:CZ    | 2.35                     | 0.62              |
| 22:DA:2504:U:C6  | 55:DA:3001:DOL:H161 | 2.33                     | 0.62              |
| 22:DA:1993:U:H4' | 25:DD:133:THR:CG2   | 2.29                     | 0.62              |
| 22:DA:2262:U:OP2 | 44:DW:16:SER:HB2    | 1.99                     | 0.62              |
| 1:AA:1504:G:OP2  | 1:AA:1507:A:O2'     | 2.16                     | 0.62              |
| 1:AA:232:G:H2'   | 1:AA:233:C:O4'      | 2.00                     | 0.62              |
| 1:AA:1226:C:OP2  | 13:AM:90:ARG:NH2    | 2.32                     | 0.62              |
| 22:BA:2192:U:C2' | 22:BA:2193:G:H5'    | 2.29                     | 0.62              |
| 22:BA:757:G:N7   | 57:BA:3304:HOH:O    | 2.31                     | 0.62              |
| 40:BS:84:ARG:HB2 | 40:BS:96:ILE:CG1    | 2.29                     | 0.62              |
| 4:CD:9:LEU:CD2   | 4:CD:22:LYS:HD2     | 2.29                     | 0.62              |
| 22:DA:223:A:C5   | 22:DA:422:A:C8      | 2.87                     | 0.62              |
| 22:DA:2550:G:C6  | 22:DA:2551:C:N4     | 2.68                     | 0.62              |
| 22:DA:450:G:N1   | 22:DA:454:A:OP2     | 2.29                     | 0.62              |
| 30:DI:6:GLN:O    | 30:DI:7:ALA:CB      | 2.48                     | 0.62              |
| 22:DA:2484:G:OP1 | 34:DM:44:ARG:NH2    | 2.32                     | 0.62              |
| 39:DR:52:PRO:O   | 39:DR:53:PHE:CG     | 2.52                     | 0.62              |
| 1:AA:1493:A:O2'  | 1:AA:1494:G:OP2     | 2.17                     | 0.62              |
| 4:AD:58:LYS:HG3  | 4:AD:59:GLN:N       | 2.13                     | 0.62              |
| 10:AJ:48:ARG:NH1 | 10:AJ:66:GLU:OE1    | 2.31                     | 0.62              |
| 22:BA:1073:A:H3' | 22:BA:1074:G:H5''   | 1.80                     | 0.62              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 22:BA:587:C:OP2    | 33:BL:21:ARG:NH1  | 2.32                     | 0.62              |
| 1:CA:1364:U:O2     | 1:CA:1364:U:H2'   | 1.99                     | 0.62              |
| 22:DA:1210:G:O6    | 22:DA:1237:A:O2'  | 2.11                     | 0.62              |
| 22:DA:1623:G:C6    | 22:DA:1624:U:C5   | 2.88                     | 0.62              |
| 22:DA:669:G:N2     | 22:DA:670:A:C2    | 2.67                     | 0.62              |
| 2:AB:186:ILE:HA    | 2:AB:200:ILE:HB   | 1.81                     | 0.62              |
| 22:BA:2188:U:H2'   | 22:BA:2189:U:C6   | 2.35                     | 0.62              |
| 32:BK:34:GLY:O     | 32:BK:35:VAL:C    | 2.37                     | 0.62              |
| 3:CC:173:VAL:O     | 3:CC:175:LEU:N    | 2.32                     | 0.62              |
| 1:CA:409:U:OP1     | 4:CD:24:GLY:CA    | 2.46                     | 0.62              |
| 18:CR:24:LYS:O     | 18:CR:26:ILE:N    | 2.32                     | 0.62              |
| 22:DA:2142:A:C2    | 22:DA:2150:C:N3   | 2.67                     | 0.62              |
| 22:DA:2407:A:OP2   | 57:DA:3558:HOH:O  | 2.15                     | 0.62              |
| 22:DA:247:G:H4'    | 22:DA:386:G:C5    | 2.34                     | 0.62              |
| 22:DA:2800:A:C2    | 22:DA:2895:G:H1'  | 2.34                     | 0.62              |
| 22:DA:511:U:H5''   | 22:DA:1235:G:H4'  | 1.81                     | 0.62              |
| 41:DT:69:ARG:NH1   | 57:DT:102:HOH:O   | 2.32                     | 0.62              |
| 13:AM:16:VAL:HG23  | 13:AM:41:GLU:O    | 2.00                     | 0.62              |
| 33:BL:61:LEU:O     | 51:B3:13:ARG:HD3  | 1.99                     | 0.62              |
| 22:BA:2066:C:OP1   | 57:BA:3512:HOH:O  | 2.16                     | 0.62              |
| 22:BA:2321:U:H5'   | 22:BA:2322:A:OP2  | 2.00                     | 0.62              |
| 25:BD:133:THR:HG23 | 25:BD:134:HIS:N   | 2.15                     | 0.62              |
| 1:CA:1007:U:H2'    | 1:CA:1008:U:H5'   | 1.81                     | 0.62              |
| 22:DA:1627:G:N2    | 22:DA:1628:G:C8   | 2.68                     | 0.62              |
| 1:AA:1446:A:H2'    | 1:AA:1447:A:H5'   | 1.81                     | 0.62              |
| 2:AB:49:MET:O      | 2:AB:53:ALA:CB    | 2.47                     | 0.62              |
| 22:BA:1246:A:C2'   | 22:BA:1247:A:O5'  | 2.48                     | 0.62              |
| 46:BY:46:VAL:O     | 46:BY:50:VAL:HG23 | 2.00                     | 0.62              |
| 1:CA:1217:C:H2'    | 1:CA:1218:C:C6    | 2.35                     | 0.62              |
| 1:CA:72:A:N6       | 1:CA:73:C:N4      | 2.48                     | 0.62              |
| 1:CA:801:U:H2'     | 1:CA:802:A:C8     | 2.35                     | 0.62              |
| 22:DA:78:U:H2'     | 22:DA:79:C:O4'    | 1.99                     | 0.62              |
| 36:DO:111:ARG:NH2  | 36:DO:117:PHE:O   | 2.33                     | 0.62              |
| 2:AB:41:ILE:HG21   | 2:AB:202:GLY:HA2  | 1.82                     | 0.62              |
| 7:AG:56:LYS:O      | 7:AG:57:SER:CB    | 2.48                     | 0.62              |
| 15:AO:2:SER:O      | 15:AO:3:LEU:CB    | 2.48                     | 0.62              |
| 22:BA:1802:A:N1    | 22:BA:1822:C:H1'  | 2.15                     | 0.62              |
| 22:BA:1838:C:C5    | 22:BA:1899:A:C5   | 2.87                     | 0.62              |
| 26:BE:106:LYS:HG3  | 26:BE:200:LEU:HG  | 1.82                     | 0.62              |
| 38:BQ:49:ASP:HA    | 38:BQ:52:GLN:HB2  | 1.81                     | 0.62              |
| 1:CA:1089:G:N2     | 1:CA:1090:U:H1'   | 2.15                     | 0.62              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:DA:2133:G:H2'   | 22:DA:2157:G:N2    | 2.14                     | 0.62              |
| 1:AA:411:A:C5      | 1:AA:429:U:C5      | 2.88                     | 0.62              |
| 2:AB:75:ALA:O      | 2:AB:76:ALA:HB2    | 2.00                     | 0.62              |
| 13:AM:64:VAL:O     | 13:AM:69:LEU:HB2   | 2.00                     | 0.62              |
| 14:AN:14:VAL:HA    | 14:AN:60:GLN:OE1   | 1.99                     | 0.62              |
| 53:B5:213:VAL:O    | 53:B5:214:TYR:CB   | 2.46                     | 0.62              |
| 22:BA:1078:U:H1'   | 22:BA:1088:A:N1    | 2.15                     | 0.62              |
| 22:BA:2327:A:H2'   | 22:BA:2328:A:C8    | 2.34                     | 0.62              |
| 22:BA:572:A:H5''   | 22:BA:573:U:OP2    | 2.00                     | 0.62              |
| 25:BD:13:ARG:HD2   | 25:BD:15:PHE:CZ    | 2.35                     | 0.62              |
| 28:BG:174:ALA:O    | 28:BG:175:LYS:CB   | 2.47                     | 0.62              |
| 1:CA:1521:C:C4     | 1:CA:1522:U:C5     | 2.87                     | 0.62              |
| 15:CO:18:ASP:OD1   | 15:CO:20:ASN:HB2   | 1.99                     | 0.62              |
| 22:DA:1582:C:O2'   | 22:DA:1585:C:N3    | 2.30                     | 0.62              |
| 22:DA:2146:C:C5'   | 22:DA:2147:A:OP1   | 2.48                     | 0.62              |
| 22:DA:237:C:C4     | 22:DA:238:C:C5     | 2.87                     | 0.62              |
| 5:AE:101:GLU:HB3   | 5:AE:122:ASN:CB    | 2.30                     | 0.62              |
| 20:AT:58:VAL:HG12  | 20:AT:59:ASP:N     | 2.14                     | 0.62              |
| 37:BP:103:ARG:CG   | 37:BP:103:ARG:HH11 | 2.13                     | 0.62              |
| 1:CA:790:A:C6      | 1:CA:791:G:C6      | 2.87                     | 0.62              |
| 2:CB:58:ASN:CG     | 2:CB:220:THR:O     | 2.37                     | 0.62              |
| 7:CG:5:ARG:HA      | 7:CG:5:ARG:NE      | 2.15                     | 0.62              |
| 9:CI:15:SER:OG     | 9:CI:69:GLY:O      | 2.10                     | 0.62              |
| 22:DA:1544:A:C6    | 22:DA:1545:A:N1    | 2.68                     | 0.62              |
| 22:DA:1827:U:O4'   | 22:DA:1970:A:O2'   | 2.17                     | 0.62              |
| 22:DA:160:A:N3     | 22:DA:2208:C:O2'   | 2.32                     | 0.62              |
| 24:DC:80:ARG:NE    | 24:DC:82:GLU:OE2   | 2.32                     | 0.62              |
| 1:AA:1366:C:O2'    | 10:AJ:62:ARG:NH2   | 2.33                     | 0.61              |
| 1:AA:723:U:H5'     | 1:AA:724:G:OP1     | 2.00                     | 0.61              |
| 10:AJ:10:LEU:CD1   | 10:AJ:98:VAL:HG12  | 2.30                     | 0.61              |
| 17:AQ:69:LYS:O     | 17:AQ:70:THR:HB    | 2.00                     | 0.61              |
| 22:BA:253:C:OP2    | 51:B3:5:LYS:HE3    | 2.00                     | 0.61              |
| 22:BA:2584:U:H2'   | 22:BA:2585:U:H5'   | 1.81                     | 0.61              |
| 22:BA:2820:A:C6    | 25:BD:197:THR:HG22 | 2.35                     | 0.61              |
| 27:BF:108:VAL:HG11 | 27:BF:176:PRO:HG2  | 1.81                     | 0.61              |
| 29:BH:93:SER:O     | 1:CA:368:U:C6      | 2.53                     | 0.61              |
| 1:CA:243:A:H4'     | 1:CA:244:U:H5''    | 1.81                     | 0.61              |
| 22:DA:1060:U:O4'   | 22:DA:1062:G:H5'   | 2.00                     | 0.61              |
| 22:DA:1248:G:N7    | 26:DE:46:GLN:NE2   | 2.47                     | 0.61              |
| 22:DA:129:C:H2'    | 22:DA:130:C:C6     | 2.35                     | 0.61              |
| 22:DA:1805:A:C2    | 22:DA:1813:G:N1    | 2.68                     | 0.61              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:DA:2726:A:O2'  | 22:DA:2727:A:O5'   | 2.18                     | 0.61              |
| 22:DA:46:G:C2     | 22:DA:47:C:C6      | 2.87                     | 0.61              |
| 22:DA:497:A:H2'   | 22:DA:498:G:O4'    | 2.00                     | 0.61              |
| 1:AA:1167:A:N7    | 1:AA:1169:A:C6     | 2.68                     | 0.61              |
| 1:AA:1491:G:H2'   | 1:AA:1492:A:O4'    | 2.00                     | 0.61              |
| 1:AA:263:A:OP2    | 20:AT:74:ARG:NH1   | 2.33                     | 0.61              |
| 1:AA:872:A:C5     | 1:AA:874:G:C8      | 2.89                     | 0.61              |
| 22:BA:1106:G:N2   | 22:BA:1107:G:H1'   | 2.15                     | 0.61              |
| 22:BA:2820:A:N1   | 25:BD:197:THR:CG2  | 2.63                     | 0.61              |
| 42:BU:18:ASP:O    | 42:BU:19:LYS:C     | 2.39                     | 0.61              |
| 43:BV:48:MET:SD   | 43:BV:86:LEU:HD12  | 2.40                     | 0.61              |
| 44:BW:68:LYS:HD3  | 44:BW:83:GLU:OE2   | 2.00                     | 0.61              |
| 1:CA:1467:C:H2'   | 1:CA:1468:A:C8     | 2.35                     | 0.61              |
| 1:CA:1417:G:C6    | 1:CA:1482:G:C6     | 2.88                     | 0.61              |
| 4:CD:29:ASP:C     | 4:CD:31:LYS:H      | 2.04                     | 0.61              |
| 7:CG:101:MET:HA   | 7:CG:104:ILE:HD12  | 1.81                     | 0.61              |
| 20:CT:67:ILE:O    | 20:CT:67:ILE:CG2   | 2.49                     | 0.61              |
| 22:DA:1855:U:C5   | 22:DA:1856:U:C5    | 2.88                     | 0.61              |
| 22:DA:200:U:C4    | 22:DA:248:G:C2     | 2.88                     | 0.61              |
| 22:DA:196:A:O2'   | 22:DA:805:G:O6     | 2.11                     | 0.61              |
| 22:DA:1790:C:O2'  | 24:DC:208:ALA:HB2  | 2.00                     | 0.61              |
| 22:DA:2590:A:O3'  | 24:DC:238:ARG:NH1  | 2.33                     | 0.61              |
| 29:DH:32:PRO:O    | 29:DH:33:GLN:CB    | 2.48                     | 0.61              |
| 1:AA:1077:G:N2    | 1:AA:1080:A:OP2    | 2.33                     | 0.61              |
| 5:AE:45:ARG:HG2   | 5:AE:73:ASN:HB3    | 1.82                     | 0.61              |
| 22:BA:1450:G:C6   | 22:BA:1451:C:N4    | 2.68                     | 0.61              |
| 22:BA:1585:C:H2'  | 22:BA:1586:A:O4'   | 1.99                     | 0.61              |
| 22:BA:319:G:C4    | 22:BA:333:G:N2     | 2.67                     | 0.61              |
| 37:BP:26:VAL:HG13 | 37:BP:47:VAL:HG23  | 1.81                     | 0.61              |
| 42:BU:16:GLY:O    | 42:BU:18:ASP:N     | 2.33                     | 0.61              |
| 1:CA:1169:A:C2    | 1:CA:1170:A:C4     | 2.88                     | 0.61              |
| 2:CB:21:ARG:HA    | 2:CB:21:ARG:NH1    | 2.16                     | 0.61              |
| 7:CG:68:ASN:ND2   | 7:CG:130:ASN:OD1   | 2.34                     | 0.61              |
| 12:CL:25:GLU:O    | 12:CL:26:ALA:C     | 2.37                     | 0.61              |
| 1:CA:728:A:C8     | 15:CO:54:ARG:CZ    | 2.83                     | 0.61              |
| 22:DA:1430:G:H2'  | 22:DA:1431:A:O4'   | 1.99                     | 0.61              |
| 28:DG:169:VAL:O   | 28:DG:169:VAL:HG12 | 2.00                     | 0.61              |
| 4:AD:26:ARG:HD2   | 4:AD:31:LYS:HE3    | 1.82                     | 0.61              |
| 19:AS:64:ASP:O    | 19:AS:65:GLU:HB3   | 2.00                     | 0.61              |
| 20:AT:3:ASN:OD1   | 20:AT:3:ASN:C      | 2.39                     | 0.61              |
| 22:BA:1028:A:N6   | 22:BA:1125:G:H2'   | 2.15                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:BA:1590:A:H2'  | 22:BA:1591:A:C8   | 2.35                     | 0.61              |
| 22:BA:528:A:C8    | 22:BA:528:A:H3'   | 2.35                     | 0.61              |
| 22:BA:877:A:N6    | 22:BA:899:A:C6    | 2.69                     | 0.61              |
| 22:BA:983:A:N6    | 22:BA:984:A:N1    | 2.49                     | 0.61              |
| 27:BF:52:ASN:CB   | 27:BF:147:ASP:OD1 | 2.49                     | 0.61              |
| 22:BA:566:U:OP1   | 33:BL:29:LYS:HD2  | 2.00                     | 0.61              |
| 22:BA:1251:C:OP2  | 38:BQ:6:ARG:HD2   | 2.00                     | 0.61              |
| 39:BR:49:ILE:HB   | 39:BR:52:PRO:O    | 1.99                     | 0.61              |
| 39:BR:14:VAL:CG1  | 39:BR:98:ILE:HG13 | 2.30                     | 0.61              |
| 1:CA:1345:U:N3    | 1:CA:1377:A:C2    | 2.68                     | 0.61              |
| 4:CD:58:LYS:NZ    | 4:CD:59:GLN:OE1   | 2.30                     | 0.61              |
| 16:CP:28:ARG:HG3  | 16:CP:29:ASN:OD1  | 2.01                     | 0.61              |
| 22:DA:1674:G:N2   | 22:DA:1677:A:H61  | 1.98                     | 0.61              |
| 22:DA:1951:U:H2'  | 22:DA:1953:A:OP2  | 2.01                     | 0.61              |
| 22:DA:242:G:O2'   | 22:DA:254:G:O6    | 2.15                     | 0.61              |
| 22:DA:425:G:N2    | 22:DA:426:C:C2    | 2.68                     | 0.61              |
| 22:DA:740:C:H5'   | 22:DA:1784:A:C3'  | 2.30                     | 0.61              |
| 22:DA:771:G:C2    | 22:DA:772:C:C6    | 2.89                     | 0.61              |
| 23:DB:29:A:H2'    | 23:DB:30:C:C6     | 2.36                     | 0.61              |
| 40:DS:67:ASP:OD1  | 40:DS:67:ASP:N    | 2.32                     | 0.61              |
| 6:AF:3:HIS:N      | 6:AF:92:THR:HG23  | 2.15                     | 0.61              |
| 22:BA:1132:U:H3'  | 22:BA:1133:A:H5'' | 1.81                     | 0.61              |
| 22:BA:1936:A:H2   | 22:BA:1943:U:H3   | 1.48                     | 0.61              |
| 38:BQ:24:TYR:O    | 38:BQ:25:TYR:HB2  | 2.00                     | 0.61              |
| 40:BS:37:THR:HG22 | 40:BS:38:TYR:CD1  | 2.35                     | 0.61              |
| 40:BS:63:GLY:O    | 40:BS:64:ALA:CB   | 2.48                     | 0.61              |
| 41:BT:67:VAL:HG22 | 41:BT:76:ARG:HG2  | 1.82                     | 0.61              |
| 1:CA:1151:A:N3    | 1:CA:1152:A:C5    | 2.68                     | 0.61              |
| 1:CA:511:C:C2     | 1:CA:512:U:C6     | 2.88                     | 0.61              |
| 6:CF:98:GLU:O     | 6:CF:99:ALA:HB3   | 2.00                     | 0.61              |
| 12:CL:47:SER:O    | 12:CL:48:ALA:HB2  | 2.01                     | 0.61              |
| 22:DA:2056:G:C2   | 22:DA:2057:G:C8   | 2.88                     | 0.61              |
| 22:DA:749:A:C5    | 22:DA:750:A:N7    | 2.69                     | 0.61              |
| 1:AA:1151:A:C4    | 1:AA:1152:A:N7    | 2.69                     | 0.61              |
| 1:AA:119:A:OP2    | 1:AA:288:A:N6     | 2.30                     | 0.61              |
| 1:AA:64:G:C8      | 1:AA:99:C:C4      | 2.89                     | 0.61              |
| 9:AI:120:LYS:HG3  | 9:AI:123:ARG:CB   | 2.31                     | 0.61              |
| 11:AK:69:ARG:CD   | 22:BA:2146:C:N3   | 2.64                     | 0.61              |
| 13:AM:74:SER:O    | 13:AM:78:LYS:HG3  | 2.01                     | 0.61              |
| 17:AQ:14:SER:HB3  | 17:AQ:22:VAL:CG1  | 2.30                     | 0.61              |
| 53:B5:184:GLU:O   | 53:B5:185:LYS:CB  | 2.49                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:BA:18:U:OP1    | 38:BQ:30:ARG:NH2  | 2.33                     | 0.61              |
| 4:CD:57:GLU:OE2   | 4:CD:196:ASN:N    | 2.34                     | 0.61              |
| 22:DA:136:G:N2    | 22:DA:144:A:N7    | 2.48                     | 0.61              |
| 1:AA:1062:U:H2'   | 1:AA:1063:C:C5    | 2.36                     | 0.61              |
| 4:AD:3:ARG:NE     | 4:AD:115:ARG:HD3  | 2.14                     | 0.61              |
| 4:AD:26:ARG:HD2   | 4:AD:31:LYS:HD2   | 1.82                     | 0.61              |
| 9:AI:43:THR:O     | 9:AI:44:ALA:HB3   | 1.99                     | 0.61              |
| 9:AI:91:ASP:OD2   | 9:AI:93:SER:N     | 2.34                     | 0.61              |
| 10:AJ:80:THR:O    | 10:AJ:82:LYS:N    | 2.33                     | 0.61              |
| 17:AQ:45:HIS:CD2  | 17:AQ:70:THR:HG23 | 2.36                     | 0.61              |
| 22:BA:1563:U:H2'  | 22:BA:1564:C:C6   | 2.36                     | 0.61              |
| 22:BA:980:A:C6    | 22:BA:981:A:N1    | 2.68                     | 0.61              |
| 35:BN:73:ASN:HA   | 35:BN:76:VAL:CG1  | 2.30                     | 0.61              |
| 38:BQ:76:TYR:OH   | 38:BQ:92:ARG:NH1  | 2.33                     | 0.61              |
| 41:BT:48:GLN:O    | 41:BT:52:GLU:HA   | 2.01                     | 0.61              |
| 1:CA:955:U:O2'    | 1:CA:1227:A:N6    | 2.33                     | 0.61              |
| 22:DA:1779:U:H5   | 22:DA:1784:A:N7   | 1.99                     | 0.61              |
| 22:DA:1868:C:N4   | 22:DA:1869:G:O6   | 2.34                     | 0.61              |
| 22:DA:2550:G:C6   | 22:DA:2551:C:C4   | 2.88                     | 0.61              |
| 22:DA:2742:G:O6   | 57:DA:3787:HOH:O  | 2.12                     | 0.61              |
| 22:DA:724:U:H2'   | 22:DA:725:G:O4'   | 2.00                     | 0.61              |
| 29:DH:83:LYS:H    | 29:DH:149:GLU:HG2 | 1.64                     | 0.61              |
| 33:DL:56:PRO:O    | 33:DL:60:ARG:HB2  | 2.00                     | 0.61              |
| 1:AA:923:A:O4'    | 1:AA:1398:A:C2    | 2.54                     | 0.61              |
| 5:AE:105:ILE:O    | 5:AE:112:ARG:NH1  | 2.33                     | 0.61              |
| 13:AM:46:SER:O    | 13:AM:47:GLU:HB3  | 2.00                     | 0.61              |
| 29:BH:97:ARG:NH1  | 1:CA:369:G:O2'    | 2.33                     | 0.61              |
| 29:BH:97:ARG:HH11 | 1:CA:370:C:H5'    | 1.66                     | 0.61              |
| 1:CA:570:G:H5''   | 1:CA:571:U:OP2    | 2.01                     | 0.61              |
| 18:CR:33:ILE:HA   | 18:CR:40:VAL:HG23 | 1.82                     | 0.61              |
| 24:DC:210:ALA:HA  | 24:DC:213:TRP:CE2 | 2.36                     | 0.61              |
| 35:DN:69:ARG:O    | 35:DN:71:ARG:N    | 2.34                     | 0.61              |
| 1:AA:448:A:C4     | 1:AA:487:A:C2     | 2.88                     | 0.61              |
| 10:AJ:33:GLY:O    | 10:AJ:34:ALA:CB   | 2.49                     | 0.61              |
| 11:AK:125:LYS:O   | 11:AK:126:LYS:O   | 2.19                     | 0.61              |
| 49:B1:28:ARG:HG2  | 49:B1:28:ARG:O    | 2.01                     | 0.61              |
| 22:BA:1131:G:OP1  | 31:BJ:82:GLY:HA2  | 2.00                     | 0.61              |
| 22:BA:1674:G:N2   | 22:BA:1677:A:N1   | 2.47                     | 0.61              |
| 32:BK:107:LEU:O   | 32:BK:109:SER:N   | 2.33                     | 0.61              |
| 22:BA:1187:G:H5'' | 39:BR:83:TYR:CE2  | 2.35                     | 0.61              |
| 1:CA:154:U:C2'    | 1:CA:155:A:H5'    | 2.31                     | 0.61              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CA:518:C:H4'    | 1:CA:519:C:O5'    | 2.00                     | 0.61              |
| 1:CA:811:C:N4     | 1:CA:812:G:C6     | 2.69                     | 0.61              |
| 6:CF:9:MET:SD     | 6:CF:59:TYR:CE1   | 2.94                     | 0.61              |
| 22:DA:467:G:OP1   | 50:D2:33:ARG:NH1  | 2.34                     | 0.61              |
| 22:DA:2001:C:H4'  | 22:DA:2689:U:H2'  | 1.82                     | 0.61              |
| 22:DA:2058:A:N6   | 22:DA:2059:A:N6   | 2.49                     | 0.61              |
| 22:DA:38:A:H2'    | 22:DA:39:G:O4'    | 2.00                     | 0.61              |
| 24:DC:16:VAL:HG22 | 24:DC:206:GLY:HA3 | 1.82                     | 0.61              |
| 25:DD:35:THR:O    | 25:DD:36:GLN:CB   | 2.49                     | 0.61              |
| 32:DK:18:ARG:HB2  | 32:DK:45:GLU:HB3  | 1.82                     | 0.61              |
| 2:AB:118:GLU:O    | 2:AB:121:SER:N    | 2.32                     | 0.61              |
| 5:AE:83:HIS:HB2   | 5:AE:84:PRO:HD2   | 1.83                     | 0.61              |
| 1:AA:1539:C:H5''  | 21:AU:18:ARG:CG   | 2.31                     | 0.61              |
| 22:BA:1014:A:C5   | 22:BA:1015:U:C5   | 2.88                     | 0.61              |
| 22:BA:142:A:C5    | 22:BA:143:C:C4    | 2.89                     | 0.61              |
| 22:BA:301:G:OP2   | 42:BU:82:ARG:NH1  | 2.34                     | 0.61              |
| 43:BV:10:LYS:HE2  | 43:BV:10:LYS:N    | 2.15                     | 0.61              |
| 46:BY:45:GLN:O    | 46:BY:46:VAL:HB   | 2.01                     | 0.61              |
| 1:CA:577:G:C8     | 1:CA:816:A:C6     | 2.89                     | 0.61              |
| 1:CA:791:G:C6     | 1:CA:792:A:N7     | 2.68                     | 0.61              |
| 2:CB:167:ASP:O    | 2:CB:168:HIS:CB   | 2.48                     | 0.61              |
| 5:CE:25:VAL:N     | 5:CE:28:GLY:O     | 2.34                     | 0.61              |
| 6:CF:69:GLU:O     | 6:CF:72:ASP:HB3   | 2.00                     | 0.61              |
| 22:DA:1360:G:C2   | 22:DA:1361:G:H1'  | 2.36                     | 0.61              |
| 22:DA:2293:G:OP1  | 22:DA:2377:A:N6   | 2.34                     | 0.61              |
| 22:DA:893:C:H2'   | 22:DA:894:U:O4'   | 2.01                     | 0.61              |
| 22:DA:636:G:N1    | 33:DL:76:GLU:OE2  | 2.33                     | 0.61              |
| 44:DW:45:PHE:CD2  | 44:DW:80:ILE:HD11 | 2.35                     | 0.61              |
| 14:AN:43:ASN:OD1  | 14:AN:47:LYS:NZ   | 2.34                     | 0.60              |
| 22:BA:1206:G:C5   | 22:BA:1207:C:C5   | 2.89                     | 0.60              |
| 22:BA:2243:U:OP1  | 57:BA:3740:HOH:O  | 2.16                     | 0.60              |
| 1:CA:718:A:N7     | 1:CA:719:C:C5     | 2.69                     | 0.60              |
| 1:CA:829:G:C6     | 1:CA:858:G:N2     | 2.69                     | 0.60              |
| 22:DA:1914:C:H3'  | 22:DA:1915:U:C6   | 2.36                     | 0.60              |
| 22:DA:200:U:C4    | 22:DA:248:G:N2    | 2.69                     | 0.60              |
| 22:DA:834:G:H1'   | 22:DA:2358:A:N3   | 2.16                     | 0.60              |
| 22:DA:353:C:H2'   | 22:DA:354:A:C8    | 2.35                     | 0.60              |
| 22:DA:56:A:C2     | 22:DA:57:C:C2     | 2.89                     | 0.60              |
| 37:DP:103:ARG:CB  | 37:DP:108:ALA:HB2 | 2.31                     | 0.60              |
| 1:AA:151:A:H2'    | 1:AA:152:A:O4'    | 2.01                     | 0.60              |
| 1:AA:792:A:N3     | 1:AA:794:A:C5     | 2.69                     | 0.60              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:AB:33:GLY:HA3   | 2:AB:40:ILE:N      | 2.16                     | 0.60              |
| 5:AE:101:GLU:CB   | 5:AE:122:ASN:HB2   | 2.31                     | 0.60              |
| 22:BA:1917:U:H2'  | 22:BA:1918:A:H5'   | 1.83                     | 0.60              |
| 22:BA:608:A:N1    | 22:BA:609:A:C2     | 2.68                     | 0.60              |
| 22:BA:1798:U:OP2  | 24:BC:271:ARG:NH2  | 2.34                     | 0.60              |
| 15:CO:17:ARG:O    | 15:CO:18:ASP:HB3   | 2.01                     | 0.60              |
| 21:CU:12:PHE:O    | 21:CU:13:ASP:HB2   | 2.01                     | 0.60              |
| 21:CU:14:VAL:HG12 | 21:CU:16:LEU:HG    | 1.83                     | 0.60              |
| 22:DA:182:A:H2'   | 22:DA:183:C:C6     | 2.36                     | 0.60              |
| 22:DA:2720:U:OP1  | 37:DP:53:ARG:NH2   | 2.35                     | 0.60              |
| 22:DA:2790:U:H5'  | 22:DA:2893:A:N7    | 2.15                     | 0.60              |
| 22:DA:43:G:N2     | 22:DA:437:U:C6     | 2.70                     | 0.60              |
| 37:DP:54:GLY:O    | 37:DP:77:HIS:NE2   | 2.34                     | 0.60              |
| 49:B1:29:THR:C    | 49:B1:31:PRO:HD3   | 2.22                     | 0.60              |
| 53:B5:99:GLU:O    | 53:B5:103:LYS:CB   | 2.50                     | 0.60              |
| 22:BA:1360:G:C6   | 22:BA:1372:U:C2    | 2.89                     | 0.60              |
| 22:BA:1923:U:O2'  | 22:BA:1924:C:C5'   | 2.49                     | 0.60              |
| 22:BA:756:A:N7    | 57:BA:3301:HOH:O   | 2.31                     | 0.60              |
| 27:BF:2:ALA:O     | 27:BF:3:LYS:C      | 2.38                     | 0.60              |
| 29:BH:121:VAL:N   | 29:BH:122:LEU:HB2  | 2.16                     | 0.60              |
| 1:CA:717:U:O2'    | 1:CA:734:G:O4'     | 2.13                     | 0.60              |
| 8:CH:10:MET:HE1   | 8:CH:36:ILE:HB     | 1.83                     | 0.60              |
| 14:CN:52:PRO:O    | 14:CN:53:ARG:CB    | 2.49                     | 0.60              |
| 22:DA:1361:G:C2   | 22:DA:1362:C:C6    | 2.88                     | 0.60              |
| 22:DA:362:A:C4    | 22:DA:363:G:C8     | 2.90                     | 0.60              |
| 37:DP:29:LYS:HB3  | 37:DP:40:LEU:HD21  | 1.83                     | 0.60              |
| 1:AA:587:G:N2     | 1:AA:755:G:C5      | 2.69                     | 0.60              |
| 4:AD:26:ARG:CD    | 4:AD:31:LYS:HD2    | 2.32                     | 0.60              |
| 22:BA:1065:U:O4   | 22:BA:1074:G:O2'   | 2.17                     | 0.60              |
| 22:BA:2318:G:C6   | 22:BA:2319:G:N1    | 2.70                     | 0.60              |
| 29:BH:100:ALA:HB1 | 29:BH:112:LYS:HA   | 1.83                     | 0.60              |
| 39:BR:29:THR:O    | 39:BR:63:VAL:HB    | 2.01                     | 0.60              |
| 1:CA:1071:C:H2'   | 1:CA:1072:G:C8     | 2.37                     | 0.60              |
| 1:CA:1240:U:OP2   | 7:CG:116:MET:N     | 2.34                     | 0.60              |
| 22:DA:1427:A:N6   | 22:DA:1571:A:OP2   | 2.35                     | 0.60              |
| 22:DA:528:A:N1    | 22:DA:2043:C:O5'   | 2.34                     | 0.60              |
| 22:DA:2645:G:H3'  | 22:DA:2646:C:H5'   | 1.83                     | 0.60              |
| 29:DH:126:GLY:O   | 29:DH:146:VAL:HG23 | 2.00                     | 0.60              |
| 1:AA:1528:U:O3'   | 1:AA:1529:G:H3'    | 2.02                     | 0.60              |
| 22:BA:1485:U:H2'  | 22:BA:1486:U:C6    | 2.36                     | 0.60              |
| 22:BA:1717:A:H2'  | 22:BA:1718:G:O5'   | 2.01                     | 0.60              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:BA:695:G:C2    | 22:BA:696:G:C8    | 2.89                     | 0.60              |
| 33:BL:68:SER:O    | 33:BL:69:ARG:CB   | 2.50                     | 0.60              |
| 1:CA:1062:U:H2'   | 1:CA:1063:C:C6    | 2.37                     | 0.60              |
| 1:CA:73:C:O2'     | 1:CA:74:A:O5'     | 2.18                     | 0.60              |
| 6:CF:36:ILE:HG12  | 6:CF:36:ILE:O     | 2.01                     | 0.60              |
| 15:CO:53:ARG:O    | 15:CO:56:LEU:N    | 2.35                     | 0.60              |
| 22:DA:1753:G:C2   | 22:DA:1756:G:N2   | 2.70                     | 0.60              |
| 22:DA:1973:G:C5   | 22:DA:1974:C:C4   | 2.89                     | 0.60              |
| 31:DJ:35:ARG:HG2  | 31:DJ:40:HIS:CD2  | 2.37                     | 0.60              |
| 38:DQ:25:TYR:CD2  | 38:DQ:26:GLY:N    | 2.69                     | 0.60              |
| 1:AA:1304:G:N1    | 1:AA:1305:G:N2    | 2.49                     | 0.60              |
| 1:AA:1391:U:H2'   | 1:AA:1392:G:C8    | 2.36                     | 0.60              |
| 1:AA:67:C:O2'     | 1:AA:171:A:N3     | 2.26                     | 0.60              |
| 1:AA:781:A:C5     | 1:AA:802:A:C2     | 2.90                     | 0.60              |
| 2:AB:154:MET:O    | 2:AB:156:GLY:N    | 2.34                     | 0.60              |
| 13:AM:114:LYS:HB2 | 13:AM:115:PRO:HD3 | 1.82                     | 0.60              |
| 1:AA:265:G:H4'    | 17:AQ:67:LEU:O    | 2.01                     | 0.60              |
| 1:AA:719:C:O2'    | 18:AR:39:ILE:O    | 2.16                     | 0.60              |
| 22:BA:1585:C:C2'  | 22:BA:1586:A:H5'  | 2.31                     | 0.60              |
| 22:BA:608:A:C6    | 22:BA:609:A:C6    | 2.90                     | 0.60              |
| 45:BX:2:SER:O     | 45:BX:4:VAL:N     | 2.34                     | 0.60              |
| 1:CA:1285:A:H4'   | 1:CA:1286:U:C5    | 2.37                     | 0.60              |
| 5:CE:157:ARG:HD3  | 5:CE:158:GLY:N    | 2.16                     | 0.60              |
| 20:CT:44:LYS:NZ   | 20:CT:86:LEU:O    | 2.31                     | 0.60              |
| 22:DA:1055:G:O2'  | 22:DA:1085:A:N1   | 2.34                     | 0.60              |
| 22:DA:1317:G:C2   | 22:DA:1336:A:C2   | 2.89                     | 0.60              |
| 22:DA:2162:G:C4'  | 22:DA:2163:A:OP1  | 2.50                     | 0.60              |
| 22:DA:2820:A:C8   | 25:DD:196:ALA:HB1 | 2.35                     | 0.60              |
| 27:DF:122:PHE:O   | 27:DF:124:GLY:N   | 2.34                     | 0.60              |
| 1:AA:1269:A:C2    | 1:AA:1313:U:O4'   | 2.54                     | 0.60              |
| 9:AI:120:LYS:HG3  | 9:AI:123:ARG:HB3  | 1.84                     | 0.60              |
| 13:AM:29:ARG:CZ   | 13:AM:63:PHE:HB2  | 2.32                     | 0.60              |
| 22:BA:2380:C:OP1  | 36:BO:17:LYS:NZ   | 2.34                     | 0.60              |
| 29:BH:117:LEU:CD2 | 29:BH:121:VAL:HA  | 2.31                     | 0.60              |
| 42:BU:49:VAL:O    | 42:BU:49:VAL:HG22 | 2.01                     | 0.60              |
| 1:CA:716:A:N3     | 11:CK:119:ASN:O   | 2.35                     | 0.60              |
| 5:CE:106:ILE:HD11 | 5:CE:124:LEU:HD23 | 1.84                     | 0.60              |
| 22:DA:1197:G:H2'  | 22:DA:1198:U:C6   | 2.37                     | 0.60              |
| 28:DG:96:ALA:N    | 28:DG:128:GLN:O   | 2.34                     | 0.60              |
| 39:DR:78:ARG:HB3  | 39:DR:83:TYR:CD1  | 2.37                     | 0.60              |
| 52:B4:24:ARG:NH1  | 52:B4:36:ARG:HD2  | 2.17                     | 0.60              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:BA:136:G:N2    | 22:BA:144:A:C5     | 2.70                     | 0.60              |
| 1:AA:702:A:N6     | 22:BA:1846:G:O2'   | 2.35                     | 0.60              |
| 24:BC:117:GLN:N   | 24:BC:128:ASN:OD1  | 2.33                     | 0.60              |
| 22:BA:1224:U:H4'  | 39:BR:88:GLY:O     | 2.00                     | 0.60              |
| 5:CE:101:GLU:O    | 5:CE:103:THR:CA    | 2.50                     | 0.60              |
| 5:CE:83:HIS:CD2   | 8:CH:96:MET:CE     | 2.84                     | 0.60              |
| 14:CN:31:ILE:O    | 14:CN:33:ASP:N     | 2.35                     | 0.60              |
| 50:D2:10:LEU:O    | 50:D2:14:ARG:HG3   | 2.02                     | 0.60              |
| 52:D4:19:ARG:O    | 52:D4:20:ASP:HB2   | 2.01                     | 0.60              |
| 22:DA:2563:U:H1'  | 22:DA:2566:A:C6    | 2.37                     | 0.60              |
| 22:DA:280:U:O4    | 22:DA:361:G:N2     | 2.35                     | 0.60              |
| 1:AA:1074:G:O2'   | 1:AA:1101:A:N1     | 2.29                     | 0.60              |
| 1:AA:1202:U:C2    | 1:AA:1203:C:C6     | 2.90                     | 0.60              |
| 4:AD:17:THR:CG2   | 4:AD:18:ASP:N      | 2.64                     | 0.60              |
| 4:AD:2:ALA:O      | 4:AD:68:LEU:HD21   | 2.02                     | 0.60              |
| 1:AA:1123:U:O2'   | 10:AJ:39:PRO:O     | 2.17                     | 0.60              |
| 22:BA:2211:A:H1'  | 22:BA:2212:A:OP1   | 2.02                     | 0.60              |
| 22:BA:2297:A:N1   | 22:BA:2321:U:C5    | 2.69                     | 0.60              |
| 22:BA:2799:A:O2'  | 22:BA:2800:A:O5'   | 2.20                     | 0.60              |
| 22:BA:278:A:C2    | 22:BA:362:A:C8     | 2.88                     | 0.60              |
| 22:BA:273:G:N2    | 22:BA:365:U:C2     | 2.69                     | 0.60              |
| 22:BA:686:U:H2'   | 22:BA:788:A:C2     | 2.36                     | 0.60              |
| 22:BA:927:A:H2'   | 22:BA:928:A:C8     | 2.37                     | 0.60              |
| 1:CA:268:U:H2'    | 1:CA:269:C:C6      | 2.36                     | 0.60              |
| 29:BH:97:ARG:NH1  | 1:CA:370:C:H5'     | 2.16                     | 0.60              |
| 1:CA:779:C:C2'    | 1:CA:780:A:H5'     | 2.32                     | 0.60              |
| 4:CD:34:ILE:O     | 4:CD:35:GLU:CB     | 2.49                     | 0.60              |
| 5:CE:137:VAL:O    | 5:CE:138:ARG:HG2   | 2.01                     | 0.60              |
| 6:CF:36:ILE:CG1   | 6:CF:36:ILE:O      | 2.49                     | 0.60              |
| 22:DA:2854:G:C2   | 22:DA:2864:G:C2    | 2.89                     | 0.60              |
| 22:DA:537:G:N1    | 22:DA:555:G:C2     | 2.70                     | 0.60              |
| 1:AA:890:G:O2'    | 1:AA:906:A:N6      | 2.34                     | 0.60              |
| 10:AJ:33:GLY:O    | 10:AJ:34:ALA:HB3   | 2.02                     | 0.60              |
| 10:AJ:53:ILE:HG22 | 10:AJ:61:ALA:HB1   | 1.84                     | 0.60              |
| 22:BA:1439:A:C2   | 22:BA:1553:A:C4    | 2.90                     | 0.60              |
| 22:BA:2318:G:C6   | 22:BA:2319:G:C6    | 2.89                     | 0.60              |
| 22:BA:1997:C:OP2  | 25:BD:129:THR:HG22 | 2.02                     | 0.60              |
| 1:CA:1151:A:C2    | 1:CA:1152:A:C6     | 2.90                     | 0.60              |
| 1:CA:154:U:H2'    | 1:CA:155:A:H5'     | 1.84                     | 0.60              |
| 1:CA:375:U:C2     | 1:CA:376:G:C8      | 2.90                     | 0.60              |
| 1:CA:388:G:O2'    | 1:CA:389:A:OP1     | 2.18                     | 0.60              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:CA:692:U:O2'    | 1:CA:694:A:N7      | 2.29                     | 0.60              |
| 4:CD:4:TYR:O      | 4:CD:5:LEU:HB2     | 2.01                     | 0.60              |
| 9:CI:57:MET:HB3   | 9:CI:61:LEU:CD2    | 2.32                     | 0.60              |
| 12:CL:21:VAL:O    | 12:CL:23:ALA:N     | 2.35                     | 0.60              |
| 22:DA:1006:C:OP2  | 57:DA:3779:HOH:O   | 2.17                     | 0.60              |
| 42:DU:18:ASP:N    | 42:DU:18:ASP:OD2   | 2.35                     | 0.60              |
| 1:AA:591:U:P      | 8:AH:31:LYS:HD2    | 2.42                     | 0.59              |
| 9:AI:113:ARG:NH2  | 14:AN:101:TRP:CZ2  | 2.69                     | 0.59              |
| 22:BA:1075:C:H2'  | 22:BA:1076:C:C2    | 2.37                     | 0.59              |
| 22:BA:1322:A:O3'  | 40:BS:84:ARG:NH1   | 2.35                     | 0.59              |
| 22:BA:1736:U:H2'  | 22:BA:1737:G:O4'   | 2.02                     | 0.59              |
| 22:BA:2444:G:P    | 26:BE:63:LYS:HD3   | 2.41                     | 0.59              |
| 32:BK:4:GLU:O     | 32:BK:5:GLN:HB2    | 2.02                     | 0.59              |
| 29:BH:93:SER:O    | 1:CA:368:U:C5      | 2.55                     | 0.59              |
| 1:CA:511:C:O2     | 1:CA:512:U:C6      | 2.55                     | 0.59              |
| 1:CA:527:G:N1     | 1:CA:528:C:C5      | 2.70                     | 0.59              |
| 22:DA:1127:A:C2'  | 22:DA:1128:G:H5''  | 2.32                     | 0.59              |
| 22:DA:118:A:N7    | 22:DA:119:A:C8     | 2.70                     | 0.59              |
| 22:DA:1875:G:C2'  | 22:DA:1876:A:OP2   | 2.50                     | 0.59              |
| 22:DA:395:U:H4'   | 22:DA:396:G:OP1    | 2.02                     | 0.59              |
| 30:DI:114:ALA:O   | 30:DI:115:ALA:CB   | 2.49                     | 0.59              |
| 31:DJ:77:HIS:HA   | 31:DJ:83:GLY:O     | 2.00                     | 0.59              |
| 42:DU:53:ASN:O    | 42:DU:53:ASN:ND2   | 2.35                     | 0.59              |
| 47:DZ:52:SER:OG   | 47:DZ:53:PHE:N     | 2.33                     | 0.59              |
| 4:AD:191:LEU:O    | 4:AD:192:SER:HB3   | 2.02                     | 0.59              |
| 4:AD:25:VAL:HG12  | 4:AD:26:ARG:N      | 2.18                     | 0.59              |
| 6:AF:63:ASN:OD1   | 6:AF:96:VAL:CG2    | 2.50                     | 0.59              |
| 24:BC:6:CYS:SG    | 24:BC:18:LYS:HD2   | 2.43                     | 0.59              |
| 27:BF:83:TYR:O    | 27:BF:85:ILE:HG22  | 2.03                     | 0.59              |
| 29:BH:99:ILE:HB   | 29:BH:115:VAL:HG11 | 1.84                     | 0.59              |
| 35:BN:49:GLU:OE2  | 35:BN:95:THR:HG22  | 2.01                     | 0.59              |
| 1:CA:577:G:C8     | 1:CA:816:A:N1      | 2.70                     | 0.59              |
| 22:DA:1109:C:H5'' | 22:DA:1110:G:OP2   | 2.01                     | 0.59              |
| 22:DA:1226:A:OP1  | 38:DQ:16:LYS:NZ    | 2.35                     | 0.59              |
| 22:DA:1436:G:C2   | 22:DA:1437:C:H1'   | 2.37                     | 0.59              |
| 22:DA:2551:C:OP2  | 57:DA:3719:HOH:O   | 2.16                     | 0.59              |
| 22:DA:2840:C:H2'  | 22:DA:2841:C:C6    | 2.37                     | 0.59              |
| 1:AA:131:A:O2'    | 1:AA:262:A:N3      | 2.32                     | 0.59              |
| 1:AA:468:A:C2     | 1:AA:469:C:C4      | 2.90                     | 0.59              |
| 10:AJ:35:GLN:HG2  | 10:AJ:77:VAL:HB    | 1.84                     | 0.59              |
| 29:BH:94:ILE:HG22 | 29:BH:99:ILE:CG1   | 2.32                     | 0.59              |

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| Atom-1            | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 33:BL:57:LEU:CD2  | 51:B3:54:ASP:HB3    | 2.33                     | 0.59              |
| 33:BL:77:ILE:HG23 | 33:BL:100:ILE:HD11  | 1.84                     | 0.59              |
| 1:CA:1072:G:C6    | 1:CA:1073:U:C4      | 2.90                     | 0.59              |
| 50:D2:44:VAL:HG13 | 50:D2:45:SER:N      | 2.17                     | 0.59              |
| 22:DA:2159:G:H2'  | 22:DA:2160:C:C6     | 2.36                     | 0.59              |
| 22:DA:2234:G:C6   | 22:DA:2235:G:N7     | 2.70                     | 0.59              |
| 22:DA:230:G:C2    | 22:DA:231:A:C8      | 2.90                     | 0.59              |
| 22:DA:2681:C:C2   | 22:DA:2724:U:O4     | 2.55                     | 0.59              |
| 22:DA:82:U:C2     | 22:DA:83:A:C8       | 2.90                     | 0.59              |
| 23:DB:37:C:C5     | 23:DB:38:C:C5       | 2.90                     | 0.59              |
| 28:DG:176:LYS:O   | 28:DG:177:LYS:HB2   | 2.02                     | 0.59              |
| 30:DI:76:ALA:CB   | 30:DI:129:ILE:HG23  | 2.33                     | 0.59              |
| 39:DR:39:LEU:HA   | 39:DR:49:ILE:HG21   | 1.83                     | 0.59              |
| 1:AA:135:C:N3     | 16:AP:1:MET:N       | 2.41                     | 0.59              |
| 1:AA:16:A:O2'     | 1:AA:17:U:H5'       | 2.03                     | 0.59              |
| 22:BA:1794:A:H2'  | 22:BA:1795:C:H6     | 1.65                     | 0.59              |
| 22:BA:2187:U:H2'  | 22:BA:2188:U:C1'    | 2.33                     | 0.59              |
| 22:BA:361:G:O2'   | 22:BA:362:A:O5'     | 2.17                     | 0.59              |
| 22:BA:877:A:C6    | 22:BA:899:A:C6      | 2.90                     | 0.59              |
| 22:BA:983:A:C6    | 22:BA:984:A:C2      | 2.90                     | 0.59              |
| 1:CA:1005:A:O3'   | 1:CA:1037:C:O2'     | 2.15                     | 0.59              |
| 1:CA:1259:C:H3'   | 1:CA:1260:G:H5''    | 1.85                     | 0.59              |
| 1:CA:992:U:C4     | 1:CA:1043:G:C8      | 2.90                     | 0.59              |
| 14:CN:61:ARG:O    | 14:CN:62:ASN:HB2    | 2.02                     | 0.59              |
| 22:DA:1688:U:C4   | 22:DA:1698:A:C2     | 2.90                     | 0.59              |
| 22:DA:2432:A:N1   | 45:DX:21:ALA:HA     | 2.17                     | 0.59              |
| 22:DA:2811:G:H2'  | 22:DA:2812:G:O4'    | 2.02                     | 0.59              |
| 23:DB:4:C:C2      | 23:DB:117:G:N2      | 2.70                     | 0.59              |
| 1:AA:1055:A:C6    | 1:AA:1206:G:C5      | 2.90                     | 0.59              |
| 1:AA:205:A:H4'    | 1:AA:205:A:OP1      | 2.01                     | 0.59              |
| 1:AA:601:G:H2'    | 1:AA:602:A:C8       | 2.37                     | 0.59              |
| 22:BA:1178:C:H2'  | 22:BA:1179:G:N7     | 2.17                     | 0.59              |
| 22:BA:1731:G:C2   | 22:BA:1733:G:C4     | 2.91                     | 0.59              |
| 22:BA:1827:U:O4   | 57:BA:3786:HOH:O    | 2.16                     | 0.59              |
| 22:BA:2017:U:H4'  | 48:B0:5:GLN:O       | 2.02                     | 0.59              |
| 22:BA:1190:G:OP1  | 33:BL:32:GLY:HA2    | 2.01                     | 0.59              |
| 6:CF:26:THR:O     | 6:CF:30:THR:OG1     | 2.20                     | 0.59              |
| 52:D4:22:VAL:O    | 52:D4:24:ARG:N      | 2.35                     | 0.59              |
| 22:DA:1343:G:H1'  | 22:DA:1597:A:C4     | 2.37                     | 0.59              |
| 22:DA:1869:G:H3'  | 22:DA:1870:C:H5'    | 1.84                     | 0.59              |
| 22:DA:2452:C:O4'  | 55:DA:3001:DOL:H461 | 2.03                     | 0.59              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:DA:396:G:C5'   | 45:DX:13:VAL:HG21  | 2.31                     | 0.59              |
| 22:DA:484:C:N4    | 22:DA:497:A:C2     | 2.70                     | 0.59              |
| 22:DA:2199:A:O4'  | 29:DH:28:ASN:ND2   | 2.36                     | 0.59              |
| 30:DI:58:VAL:CG1  | 30:DI:59:ILE:N     | 2.65                     | 0.59              |
| 1:AA:1378:C:C5    | 1:AA:1379:G:C8     | 2.91                     | 0.59              |
| 1:AA:587:G:C2     | 1:AA:755:G:C5      | 2.90                     | 0.59              |
| 9:AI:63:LEU:HD23  | 9:AI:63:LEU:N      | 2.17                     | 0.59              |
| 18:AR:67:LEU:O    | 18:AR:68:LEU:HG    | 2.02                     | 0.59              |
| 20:AT:70:ASN:N    | 20:AT:70:ASN:OD1   | 2.28                     | 0.59              |
| 22:BA:1045:C:C3'  | 22:BA:1046:A:H5'   | 2.32                     | 0.59              |
| 22:BA:1359:A:C8   | 22:BA:1373:A:C2    | 2.91                     | 0.59              |
| 22:BA:2714:G:C2'  | 22:BA:2715:C:H5'   | 2.32                     | 0.59              |
| 22:BA:947:A:HO2'  | 22:BA:984:A:H2     | 1.42                     | 0.59              |
| 24:BC:204:VAL:O   | 24:BC:205:LEU:HB2  | 2.02                     | 0.59              |
| 18:CR:63:ARG:HB3  | 18:CR:70:TYR:CE1   | 2.37                     | 0.59              |
| 22:DA:1315:C:OP2  | 57:DA:3760:HOH:O   | 2.16                     | 0.59              |
| 22:DA:424:G:C2    | 22:DA:425:G:C8     | 2.90                     | 0.59              |
| 22:DA:861:A:H2'   | 22:DA:862:G:O4'    | 2.02                     | 0.59              |
| 29:DH:126:GLY:O   | 29:DH:146:VAL:N    | 2.35                     | 0.59              |
| 36:DO:64:TYR:O    | 36:DO:67:ASN:ND2   | 2.33                     | 0.59              |
| 1:AA:1157:A:N6    | 1:AA:1180:A:N7     | 2.51                     | 0.59              |
| 1:AA:345:C:O2'    | 32:BK:116:ILE:HD11 | 2.02                     | 0.59              |
| 14:AN:41:ARG:O    | 14:AN:43:ASN:N     | 2.36                     | 0.59              |
| 52:B4:36:ARG:HG2  | 52:B4:37:GLN:N     | 2.16                     | 0.59              |
| 22:BA:1735:A:C2   | 22:BA:1736:U:C1'   | 2.86                     | 0.59              |
| 22:BA:1867:G:O2'  | 22:BA:1868:C:H5'   | 2.02                     | 0.59              |
| 29:BH:1:MET:O     | 29:BH:20:ASN:ND2   | 2.35                     | 0.59              |
| 40:BS:29:VAL:CG1  | 40:BS:55:ILE:HD11  | 2.32                     | 0.59              |
| 1:CA:1309:G:C6    | 1:CA:1329:A:C2     | 2.90                     | 0.59              |
| 1:CA:518:C:H5''   | 1:CA:519:C:C6      | 2.37                     | 0.59              |
| 12:CL:18:LYS:HD2  | 12:CL:18:LYS:C     | 2.23                     | 0.59              |
| 22:DA:1364:G:H2'  | 22:DA:1365:A:H5'   | 1.84                     | 0.59              |
| 22:DA:9:G:C6      | 22:DA:2629:U:C6    | 2.91                     | 0.59              |
| 42:DU:72:ILE:HD13 | 42:DU:83:VAL:CG2   | 2.32                     | 0.59              |
| 1:AA:1134:G:C2    | 1:AA:1135:U:C2     | 2.90                     | 0.59              |
| 10:AJ:17:LEU:HD23 | 10:AJ:17:LEU:C     | 2.22                     | 0.59              |
| 15:AO:87:LEU:O    | 15:AO:88:ARG:CB    | 2.50                     | 0.59              |
| 22:BA:1199:U:H2'  | 22:BA:1200:C:C6    | 2.38                     | 0.59              |
| 22:BA:1768:C:C2   | 22:BA:1769:U:C6    | 2.90                     | 0.59              |
| 22:BA:2191:A:C2   | 22:BA:2192:U:C4    | 2.91                     | 0.59              |
| 34:BM:24:THR:HG23 | 34:BM:24:THR:O     | 2.01                     | 0.59              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:CA:1211:U:C2'   | 1:CA:1212:U:OP2    | 2.51                     | 0.59              |
| 1:CA:33:A:H2'     | 1:CA:34:C:H6       | 1.67                     | 0.59              |
| 1:CA:411:A:C5     | 1:CA:429:U:C5      | 2.91                     | 0.59              |
| 1:CA:254:G:O2'    | 17:CQ:18:GLU:O     | 2.20                     | 0.59              |
| 48:D0:55:ILE:O    | 48:D0:56:ALA:HB3   | 2.03                     | 0.59              |
| 22:DA:1773:A:N3   | 22:DA:1978:A:C2    | 2.71                     | 0.59              |
| 22:DA:2343:U:O2'  | 22:DA:2373:G:O2'   | 2.19                     | 0.59              |
| 30:DI:58:VAL:O    | 30:DI:69:PHE:HB3   | 2.03                     | 0.59              |
| 1:AA:328:C:O2     | 1:AA:328:C:H2'     | 2.01                     | 0.59              |
| 1:AA:760:G:N7     | 1:AA:761:G:C8      | 2.71                     | 0.59              |
| 20:AT:6:SER:OG    | 20:AT:7:ALA:N      | 2.36                     | 0.59              |
| 22:BA:1406:U:C2   | 22:BA:1407:G:C8    | 2.91                     | 0.59              |
| 22:BA:142:A:H2'   | 22:BA:143:C:C6     | 2.38                     | 0.59              |
| 30:BI:117:MET:HE3 | 30:BI:129:ILE:HD11 | 1.84                     | 0.59              |
| 32:BK:121:GLU:O   | 32:BK:122:VAL:O    | 2.21                     | 0.59              |
| 39:BR:49:ILE:CG2  | 39:BR:53:PHE:N     | 2.65                     | 0.59              |
| 1:CA:55:A:C6      | 1:CA:56:U:C2       | 2.91                     | 0.59              |
| 12:CL:68:GLY:O    | 12:CL:99:ARG:NH1   | 2.36                     | 0.59              |
| 21:CU:8:GLU:HB3   | 21:CU:12:PHE:CD2   | 2.38                     | 0.59              |
| 22:DA:1753:G:C2   | 22:DA:1756:G:C2    | 2.90                     | 0.59              |
| 22:DA:532:A:N1    | 22:DA:2020:A:H1'   | 2.18                     | 0.59              |
| 22:DA:53:A:N7     | 22:DA:54:G:C5      | 2.71                     | 0.59              |
| 1:AA:340:U:C2     | 1:AA:341:C:C5      | 2.91                     | 0.59              |
| 1:AA:340:U:H2'    | 1:AA:341:C:H6      | 1.67                     | 0.59              |
| 5:AE:46:VAL:CG2   | 5:AE:118:ALA:HA    | 2.33                     | 0.59              |
| 16:AP:42:ILE:O    | 16:AP:43:ALA:C     | 2.41                     | 0.59              |
| 22:BA:142:A:N7    | 22:BA:143:C:N4     | 2.51                     | 0.59              |
| 22:BA:2495:G:C2'  | 22:BA:2496:C:H5'   | 2.33                     | 0.59              |
| 27:BF:106:ILE:C   | 27:BF:109:PRO:HD2  | 2.22                     | 0.59              |
| 40:BS:84:ARG:HB2  | 40:BS:96:ILE:HG13  | 1.85                     | 0.59              |
| 1:CA:214:C:H2'    | 1:CA:215:C:C6      | 2.37                     | 0.59              |
| 22:DA:1121:C:C2   | 22:DA:1122:G:C8    | 2.91                     | 0.59              |
| 22:DA:2297:A:N1   | 22:DA:2321:U:C5    | 2.71                     | 0.59              |
| 26:DE:47:LYS:O    | 26:DE:83:VAL:HB    | 2.03                     | 0.59              |
| 31:DJ:9:GLU:O     | 31:DJ:10:THR:HG23  | 2.03                     | 0.59              |
| 1:AA:68:G:C5      | 1:AA:69:G:H1'      | 2.38                     | 0.58              |
| 5:AE:101:GLU:HB3  | 5:AE:122:ASN:HB2   | 1.84                     | 0.58              |
| 10:AJ:53:ILE:HG22 | 10:AJ:61:ALA:CB    | 2.33                     | 0.58              |
| 11:AK:16:VAL:HG22 | 11:AK:17:SER:N     | 2.18                     | 0.58              |
| 22:BA:1084:A:H2'  | 22:BA:1085:A:C8    | 2.38                     | 0.58              |
| 22:BA:1167:C:H2'  | 22:BA:1168:G:H5''  | 1.85                     | 0.58              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 22:BA:644:A:H2'  | 22:BA:645:C:O4'   | 2.03                     | 0.58              |
| 22:BA:783:A:C8   | 22:BA:784:G:H4'   | 2.38                     | 0.58              |
| 22:BA:784:G:OP2  | 57:BA:3313:HOH:O  | 2.16                     | 0.58              |
| 1:CA:1006:G:H2'  | 1:CA:1007:U:C6    | 2.38                     | 0.58              |
| 1:CA:152:A:N6    | 1:CA:170:U:C2     | 2.71                     | 0.58              |
| 2:CB:134:ALA:O   | 2:CB:138:THR:OG1  | 2.08                     | 0.58              |
| 2:CB:47:VAL:HB   | 2:CB:48:PRO:HD3   | 1.84                     | 0.58              |
| 9:CI:57:MET:SD   | 9:CI:58:VAL:N     | 2.76                     | 0.58              |
| 21:CU:14:VAL:O   | 21:CU:16:LEU:HG   | 2.03                     | 0.58              |
| 21:CU:15:ALA:O   | 21:CU:17:ARG:N    | 2.36                     | 0.58              |
| 22:DA:1304:A:N1  | 22:DA:1305:C:C4   | 2.72                     | 0.58              |
| 22:DA:2111:U:C4  | 22:DA:2145:C:H2'  | 2.39                     | 0.58              |
| 22:DA:20:C:H2'   | 22:DA:21:A:C8     | 2.38                     | 0.58              |
| 22:DA:454:A:H4'  | 22:DA:455:C:OP2   | 2.01                     | 0.58              |
| 22:DA:777:G:N7   | 22:DA:793:A:H2    | 2.00                     | 0.58              |
| 22:DA:856:G:C2   | 22:DA:922:C:N3    | 2.71                     | 0.58              |
| 23:DB:87:U:O2'   | 23:DB:88:C:H5'    | 2.02                     | 0.58              |
| 1:AA:152:A:N6    | 1:AA:170:U:C2     | 2.70                     | 0.58              |
| 1:AA:792:A:H1'   | 1:AA:794:A:N7     | 2.18                     | 0.58              |
| 10:AJ:15:HIS:O   | 10:AJ:17:LEU:N    | 2.32                     | 0.58              |
| 21:AU:4:ILE:N    | 21:AU:20:LYS:HZ1  | 2.01                     | 0.58              |
| 49:B1:4:GLY:O    | 49:B1:6:ARG:N     | 2.37                     | 0.58              |
| 22:BA:481:G:N3   | 22:BA:507:A:C2    | 2.71                     | 0.58              |
| 24:BC:167:ARG:O  | 24:BC:168:ASP:HB2 | 2.03                     | 0.58              |
| 36:BO:15:ARG:NE  | 36:BO:93:ASP:OD1  | 2.36                     | 0.58              |
| 1:CA:1499:A:H3'  | 57:CA:1884:HOH:O  | 2.02                     | 0.58              |
| 1:CA:570:G:H1'   | 1:CA:820:U:C4     | 2.38                     | 0.58              |
| 1:CA:920:U:H2'   | 1:CA:921:U:C6     | 2.36                     | 0.58              |
| 1:CA:994:A:N3    | 1:CA:994:A:H2'    | 2.17                     | 0.58              |
| 2:CB:133:GLU:O   | 2:CB:137:ARG:HB3  | 2.03                     | 0.58              |
| 5:CE:56:VAL:O    | 5:CE:60:ILE:HG23  | 2.03                     | 0.58              |
| 17:CQ:47:HIS:HB2 | 17:CQ:67:LEU:HD12 | 1.85                     | 0.58              |
| 20:CT:55:GLN:N   | 20:CT:56:PRO:CD   | 2.65                     | 0.58              |
| 22:DA:1380:G:OP2 | 57:DA:3751:HOH:O  | 2.17                     | 0.58              |
| 22:DA:2074:U:H2' | 22:DA:2075:U:C6   | 2.38                     | 0.58              |
| 22:DA:308:G:N1   | 22:DA:309:A:C2    | 2.70                     | 0.58              |
| 22:DA:307:G:N2   | 22:DA:310:A:C8    | 2.71                     | 0.58              |
| 22:DA:319:G:O6   | 22:DA:323:C:N4    | 2.35                     | 0.58              |
| 22:DA:2746:U:H1' | 28:DG:139:GLN:HG3 | 1.85                     | 0.58              |
| 2:AB:147:SER:O   | 2:AB:148:LEU:CB   | 2.51                     | 0.58              |
| 4:AD:68:LEU:HD22 | 4:AD:68:LEU:N     | 2.18                     | 0.58              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:AD:78:GLU:OE1    | 4:AD:81:ARG:NH1    | 2.37                     | 0.58              |
| 14:AN:21:PHE:HA    | 14:AN:25:ALA:CB    | 2.33                     | 0.58              |
| 22:BA:257:C:H5''   | 22:BA:258:G:OP2    | 2.03                     | 0.58              |
| 22:BA:973:A:O4'    | 22:BA:1188:U:C6    | 2.56                     | 0.58              |
| 25:BD:133:THR:HG23 | 25:BD:134:HIS:CD2  | 2.38                     | 0.58              |
| 22:BA:2578:G:N7    | 25:BD:145:SER:HB2  | 2.18                     | 0.58              |
| 25:BD:151:THR:HG22 | 25:BD:152:PRO:HD2  | 1.84                     | 0.58              |
| 27:BF:143:TYR:O    | 27:BF:146:VAL:HG22 | 2.03                     | 0.58              |
| 32:BK:116:ILE:O    | 32:BK:118:LEU:O    | 2.21                     | 0.58              |
| 1:CA:1108:G:H5''   | 3:CC:176:HIS:CD2   | 2.37                     | 0.58              |
| 1:CA:994:A:C8      | 1:CA:1216:A:H4'    | 2.39                     | 0.58              |
| 1:CA:692:U:H1'     | 1:CA:695:A:N7      | 2.19                     | 0.58              |
| 1:CA:755:G:C2      | 1:CA:756:C:C5      | 2.91                     | 0.58              |
| 2:CB:90:PHE:CZ     | 2:CB:154:MET:HA    | 2.38                     | 0.58              |
| 4:CD:35:GLU:O      | 4:CD:38:PRO:HD3    | 2.02                     | 0.58              |
| 11:CK:126:LYS:O    | 11:CK:127:ARG:HB2  | 2.03                     | 0.58              |
| 17:CQ:46:VAL:HG21  | 17:CQ:61:ILE:CD1   | 2.34                     | 0.58              |
| 22:DA:120:U:H1'    | 22:DA:149:A:C8     | 2.37                     | 0.58              |
| 22:DA:2104:C:H2'   | 22:DA:2105:U:O4'   | 2.04                     | 0.58              |
| 22:DA:2182:U:H2'   | 22:DA:2183:A:C8    | 2.38                     | 0.58              |
| 22:DA:2334:U:C4    | 36:DO:16:ARG:HD3   | 2.38                     | 0.58              |
| 22:DA:2857:G:N2    | 22:DA:2860:A:OP2   | 2.34                     | 0.58              |
| 22:DA:847:U:O2     | 22:DA:847:U:H2'    | 2.03                     | 0.58              |
| 27:DF:122:PHE:CE1  | 27:DF:166:GLY:HA3  | 2.38                     | 0.58              |
| 46:DY:56:LEU:O     | 46:DY:57:LEU:HB2   | 2.04                     | 0.58              |
| 1:AA:1107:C:C4     | 1:AA:1108:G:N7     | 2.72                     | 0.58              |
| 1:AA:1171:A:C2     | 1:AA:1172:C:C2     | 2.92                     | 0.58              |
| 2:AB:133:GLU:O     | 2:AB:137:ARG:HB2   | 2.03                     | 0.58              |
| 5:AE:137:VAL:O     | 5:AE:138:ARG:CB    | 2.51                     | 0.58              |
| 8:AH:113:ASP:OD2   | 8:AH:117:ARG:NH2   | 2.36                     | 0.58              |
| 21:AU:4:ILE:N      | 21:AU:19:PHE:CD1   | 2.71                     | 0.58              |
| 22:BA:1361:G:N7    | 57:BA:3618:HOH:O   | 2.32                     | 0.58              |
| 22:BA:1696:G:C6    | 22:BA:1697:G:C4    | 2.91                     | 0.58              |
| 27:BF:123:ASP:OD2  | 27:BF:127:ASN:HB2  | 2.02                     | 0.58              |
| 1:CA:960:U:C5      | 1:CA:1225:A:C8     | 2.91                     | 0.58              |
| 1:CA:190:A:C8      | 1:CA:191:G:H1'     | 2.38                     | 0.58              |
| 1:CA:257:G:C2      | 1:CA:270:A:N1      | 2.71                     | 0.58              |
| 1:CA:681:A:C2      | 1:CA:710:G:C2      | 2.92                     | 0.58              |
| 1:CA:765:G:C6      | 1:CA:812:G:C4      | 2.92                     | 0.58              |
| 4:CD:30:THR:C      | 4:CD:31:LYS:HD3    | 2.23                     | 0.58              |
| 5:CE:122:ASN:O     | 5:CE:123:VAL:O     | 2.22                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:DA:1091:G:N3   | 22:DA:1092:C:C5   | 2.71                     | 0.58              |
| 22:DA:1606:C:O2'  | 22:DA:1607:C:OP2  | 2.19                     | 0.58              |
| 22:DA:2744:G:C6   | 22:DA:2761:A:N6   | 2.72                     | 0.58              |
| 22:DA:546:U:O2'   | 22:DA:547:A:O4'   | 2.21                     | 0.58              |
| 23:DB:7:G:H5'     | 36:DO:29:HIS:CE1  | 2.38                     | 0.58              |
| 23:DB:78:A:C6     | 23:DB:99:A:C8     | 2.90                     | 0.58              |
| 1:AA:1211:U:HO2'  | 1:AA:1212:U:P     | 2.26                     | 0.58              |
| 1:AA:524:G:H5''   | 1:AA:525:C:OP2    | 2.02                     | 0.58              |
| 1:AA:596:A:C6     | 1:AA:645:G:C2     | 2.92                     | 0.58              |
| 2:AB:151:ILE:HG23 | 2:AB:152:LYS:N    | 2.18                     | 0.58              |
| 3:AC:206:GLU:O    | 3:AC:207:ILE:HG22 | 2.03                     | 0.58              |
| 14:AN:49:GLN:OE1  | 14:AN:49:GLN:HA   | 2.03                     | 0.58              |
| 22:BA:1095:A:C6   | 22:BA:1096:A:N6   | 2.71                     | 0.58              |
| 22:BA:999:U:C5    | 22:BA:1154:G:C5   | 2.91                     | 0.58              |
| 22:BA:1915:U:C2'  | 22:BA:1916:A:H5'  | 2.33                     | 0.58              |
| 22:BA:871:U:H2'   | 22:BA:872:U:C6    | 2.38                     | 0.58              |
| 24:BC:70:ASN:O    | 24:BC:71:LYS:C    | 2.41                     | 0.58              |
| 37:BP:90:GLY:O    | 37:BP:113:ARG:NH1 | 2.37                     | 0.58              |
| 1:CA:1343:G:H2'   | 1:CA:1344:C:C6    | 2.39                     | 0.58              |
| 1:CA:373:A:C2     | 1:CA:374:A:C8     | 2.91                     | 0.58              |
| 1:CA:728:A:H2'    | 1:CA:729:A:C8     | 2.38                     | 0.58              |
| 2:CB:120:GLN:HG2  | 2:CB:125:THR:O    | 2.03                     | 0.58              |
| 22:DA:2128:G:N3   | 22:DA:2173:A:O2'  | 2.36                     | 0.58              |
| 22:DA:1154:G:OP2  | 38:DQ:58:ARG:NH1  | 2.36                     | 0.58              |
| 1:AA:108:G:N3     | 1:AA:108:G:H5'    | 2.19                     | 0.58              |
| 1:AA:212:G:C2     | 1:AA:213:G:C4     | 2.91                     | 0.58              |
| 1:AA:4:U:O2       | 1:AA:4:U:H2'      | 2.04                     | 0.58              |
| 11:AK:31:ILE:HB   | 11:AK:46:THR:HG22 | 1.85                     | 0.58              |
| 12:AL:24:LEU:HB2  | 12:AL:59:ASN:ND2  | 2.18                     | 0.58              |
| 15:AO:63:ARG:CG   | 15:AO:67:LEU:HD12 | 2.33                     | 0.58              |
| 22:BA:123:G:N7    | 57:BA:3213:HOH:O  | 2.32                     | 0.58              |
| 1:AA:1492:A:O2'   | 22:BA:1913:A:N1   | 2.27                     | 0.58              |
| 22:BA:1916:A:H2'  | 22:BA:1917:U:O2'  | 2.04                     | 0.58              |
| 22:BA:2564:A:C2   | 22:BA:2647:U:H4'  | 2.38                     | 0.58              |
| 27:BF:171:ALA:O   | 27:BF:174:ASP:N   | 2.36                     | 0.58              |
| 29:BH:31:VAL:N    | 29:BH:32:PRO:HD2  | 2.19                     | 0.58              |
| 34:BM:12:MET:HE3  | 34:BM:71:LYS:HG3  | 1.86                     | 0.58              |
| 47:BZ:11:ARG:NH1  | 47:BZ:53:PHE:O    | 2.37                     | 0.58              |
| 1:CA:938:A:N6     | 1:CA:939:G:C6     | 2.71                     | 0.58              |
| 2:CB:119:THR:O    | 2:CB:120:GLN:CB   | 2.52                     | 0.58              |
| 22:DA:1363:C:H2'  | 22:DA:1364:G:H8   | 1.69                     | 0.58              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:DA:1640:A:H2'  | 22:DA:1641:A:C8   | 2.39                     | 0.58              |
| 22:DA:2314:A:C2   | 22:DA:2315:G:C4   | 2.91                     | 0.58              |
| 22:DA:2883:A:OP2  | 48:D0:49:TYR:OH   | 2.18                     | 0.58              |
| 22:DA:607:U:N3    | 22:DA:620:G:O4'   | 2.36                     | 0.58              |
| 31:DJ:110:PRO:O   | 31:DJ:115:GLY:HA3 | 2.03                     | 0.58              |
| 31:DJ:19:ASP:O    | 31:DJ:23:LYS:HE3  | 2.03                     | 0.58              |
| 31:DJ:30:THR:HG22 | 31:DJ:31:GLU:N    | 2.18                     | 0.58              |
| 1:AA:1362:A:H5''  | 1:AA:1363:A:OP2   | 2.03                     | 0.58              |
| 1:AA:572:A:H5'    | 1:AA:573:A:OP2    | 2.02                     | 0.58              |
| 1:AA:577:G:C8     | 1:AA:816:A:C6     | 2.91                     | 0.58              |
| 1:AA:757:U:O2'    | 1:AA:879:C:O2     | 2.21                     | 0.58              |
| 22:BA:1405:U:H2'  | 22:BA:1406:U:C6   | 2.39                     | 0.58              |
| 22:BA:1423:G:O6   | 57:BA:3628:HOH:O  | 2.17                     | 0.58              |
| 22:BA:1916:A:P    | 22:BA:1917:U:OP2  | 2.62                     | 0.58              |
| 30:BI:62:TYR:O    | 30:BI:63:ALA:CB   | 2.51                     | 0.58              |
| 1:CA:1381:U:H2'   | 1:CA:1382:C:O5'   | 2.04                     | 0.58              |
| 1:CA:17:U:C2      | 1:CA:18:C:C5      | 2.92                     | 0.58              |
| 4:CD:29:ASP:C     | 4:CD:31:LYS:N     | 2.56                     | 0.58              |
| 12:CL:44:LYS:O    | 12:CL:46:ASN:N    | 2.37                     | 0.58              |
| 22:DA:1075:C:H2'  | 22:DA:1076:C:C6   | 2.39                     | 0.58              |
| 22:DA:1062:G:C5   | 22:DA:1088:A:H2'  | 2.39                     | 0.58              |
| 22:DA:30:G:O2'    | 22:DA:1214:A:N3   | 2.36                     | 0.58              |
| 22:DA:150:U:H2'   | 22:DA:151:C:C6    | 2.38                     | 0.58              |
| 22:DA:2563:U:C1'  | 22:DA:2566:A:N6   | 2.65                     | 0.58              |
| 22:DA:453:A:H4'   | 22:DA:472:A:N6    | 2.17                     | 0.58              |
| 22:DA:699:A:H2'   | 22:DA:700:G:O4'   | 2.04                     | 0.58              |
| 22:DA:699:A:N6    | 22:DA:733:G:O2'   | 2.36                     | 0.58              |
| 29:DH:34:GLY:O    | 29:DH:35:LYS:CB   | 2.51                     | 0.58              |
| 17:AQ:45:HIS:CD2  | 17:AQ:70:THR:CG2  | 2.87                     | 0.58              |
| 22:BA:1206:G:C6   | 22:BA:1207:C:C4   | 2.92                     | 0.58              |
| 22:BA:1253:A:N7   | 57:BA:3337:HOH:O  | 2.32                     | 0.58              |
| 22:BA:1593:A:H2'  | 22:BA:1594:U:O4'  | 2.03                     | 0.58              |
| 22:BA:1624:U:N3   | 22:BA:1625:C:C5   | 2.72                     | 0.58              |
| 22:BA:580:U:O3'   | 38:BQ:31:VAL:HG13 | 2.04                     | 0.58              |
| 22:BA:674:G:O2'   | 26:BE:69:ARG:HB3  | 2.03                     | 0.58              |
| 39:BR:9:GLY:C     | 39:BR:10:LYS:HG2  | 2.24                     | 0.58              |
| 1:CA:1027:C:N4    | 1:CA:1034:G:C6    | 2.72                     | 0.58              |
| 1:CA:649:A:H2'    | 1:CA:650:G:O4'    | 2.04                     | 0.58              |
| 5:CE:109:GLY:O    | 5:CE:110:ALA:HB3  | 2.04                     | 0.58              |
| 19:CS:31:LEU:O    | 19:CS:33:THR:N    | 2.36                     | 0.58              |
| 22:DA:126:A:N7    | 22:DA:127:A:C2    | 2.72                     | 0.58              |

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| Atom-1            | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 22:DA:2330:G:N2   | 22:DA:2386:A:C2     | 2.71                     | 0.58              |
| 22:DA:53:A:N3     | 22:DA:179:C:H4'     | 2.18                     | 0.58              |
| 24:DC:108:LYS:N   | 24:DC:194:GLU:O     | 2.36                     | 0.58              |
| 25:DD:123:LYS:HG2 | 25:DD:165:MET:SD    | 2.44                     | 0.58              |
| 28:DG:27:LYS:O    | 28:DG:27:LYS:HG3    | 2.03                     | 0.58              |
| 31:DJ:78:THR:OG1  | 31:DJ:80:HIS:HB2    | 2.04                     | 0.58              |
| 34:DM:76:LYS:NZ   | 34:DM:85:GLY:O      | 2.37                     | 0.58              |
| 39:DR:14:VAL:HG21 | 39:DR:98:ILE:HG13   | 1.84                     | 0.58              |
| 41:DT:82:LYS:HG2  | 41:DT:83:ALA:N      | 2.18                     | 0.58              |
| 1:AA:1306:A:C4    | 1:AA:1307:U:C6      | 2.92                     | 0.58              |
| 1:AA:568:G:C4     | 1:AA:569:C:C5       | 2.92                     | 0.58              |
| 1:AA:684:U:HO2'   | 11:AK:40:ASN:C      | 2.05                     | 0.58              |
| 1:AA:760:G:C5     | 1:AA:761:G:C8       | 2.92                     | 0.58              |
| 5:AE:25:VAL:O     | 5:AE:27:GLY:N       | 2.37                     | 0.58              |
| 48:B0:55:ILE:HG22 | 48:B0:56:ALA:N      | 2.18                     | 0.58              |
| 30:BI:79:LEU:HD22 | 30:BI:109:ILE:CG2   | 2.34                     | 0.58              |
| 30:BI:81:LYS:HA   | 30:BI:86:ILE:O      | 2.03                     | 0.58              |
| 31:BJ:17:VAL:HG23 | 31:BJ:137:PRO:HB2   | 1.85                     | 0.58              |
| 36:BO:100:HIS:O   | 36:BO:104:GLN:CB    | 2.52                     | 0.58              |
| 46:BY:23:ARG:O    | 46:BY:24:GLU:C      | 2.42                     | 0.58              |
| 1:CA:1167:A:N7    | 1:CA:1169:A:C6      | 2.71                     | 0.58              |
| 1:CA:115:G:H4'    | 1:CA:116:A:O5'      | 2.04                     | 0.58              |
| 1:CA:624:C:H2'    | 1:CA:625:U:O4'      | 2.04                     | 0.58              |
| 4:CD:9:LEU:HD12   | 4:CD:32:CYS:SG      | 2.43                     | 0.58              |
| 6:CF:97:THR:O     | 6:CF:98:GLU:HB3     | 2.04                     | 0.58              |
| 20:CT:15:GLU:OE2  | 20:CT:18:ARG:NH2    | 2.35                     | 0.58              |
| 20:CT:67:ILE:HG22 | 20:CT:67:ILE:O      | 2.03                     | 0.58              |
| 22:DA:2328:A:H2'  | 22:DA:2329:U:C6     | 2.38                     | 0.58              |
| 22:DA:2552:U:C2   | 22:DA:2554:U:H5'    | 2.39                     | 0.58              |
| 22:DA:647:G:C5    | 22:DA:648:G:N7      | 2.71                     | 0.58              |
| 42:DU:13:VAL:HG21 | 42:DU:39:ILE:CG2    | 2.33                     | 0.58              |
| 1:AA:475:C:H2'    | 1:AA:476:U:O4'      | 2.04                     | 0.58              |
| 1:AA:721:G:H4'    | 1:AA:722:G:O4'      | 2.03                     | 0.58              |
| 8:AH:125:ILE:O    | 8:AH:125:ILE:HG13   | 2.04                     | 0.58              |
| 21:AU:37:PHE:HB3  | 21:AU:41:PRO:CG     | 2.34                     | 0.58              |
| 22:BA:1022:G:N2   | 22:BA:1142:A:C2     | 2.71                     | 0.58              |
| 22:BA:1563:U:H2'  | 22:BA:1564:C:H6     | 1.69                     | 0.58              |
| 22:BA:2192:U:C4   | 22:BA:2193:G:C8     | 2.92                     | 0.58              |
| 22:BA:2584:U:O2'  | 55:BA:3001:DOL:H482 | 2.03                     | 0.58              |
| 22:BA:481:G:H1'   | 22:BA:507:A:N1      | 2.19                     | 0.58              |
| 22:BA:603:A:C8    | 22:BA:655:A:C6      | 2.92                     | 0.58              |

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| Atom-1            | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 22:BA:65:U:H2'    | 22:BA:66:C:H6       | 1.68                     | 0.58              |
| 22:BA:846:U:O2'   | 22:BA:847:U:P       | 2.62                     | 0.58              |
| 22:BA:1248:G:C6   | 26:BE:46:GLN:NE2    | 2.72                     | 0.58              |
| 27:BF:108:VAL:N   | 27:BF:109:PRO:CD    | 2.66                     | 0.58              |
| 39:BR:51:VAL:O    | 39:BR:52:PRO:O      | 2.22                     | 0.58              |
| 41:BT:34:VAL:HG21 | 41:BT:43:ILE:HD11   | 1.85                     | 0.58              |
| 3:CC:72:ARG:HB3   | 3:CC:75:ILE:HG23    | 1.85                     | 0.58              |
| 6:CF:43:GLY:HA2   | 6:CF:58:HIS:NE2     | 2.19                     | 0.58              |
| 10:CJ:84:VAL:O    | 10:CJ:88:MET:HB2    | 2.04                     | 0.58              |
| 12:CL:21:VAL:N    | 12:CL:22:PRO:HD3    | 2.19                     | 0.58              |
| 22:DA:1551:A:N6   | 57:DA:3628:HOH:O    | 2.35                     | 0.58              |
| 22:DA:1806:C:C5   | 22:DA:1807:G:N7     | 2.72                     | 0.58              |
| 22:DA:1817:G:H2'  | 22:DA:1818:U:H5'    | 1.86                     | 0.58              |
| 22:DA:2061:G:C5   | 55:DA:3001:DOL:HC19 | 2.38                     | 0.58              |
| 22:DA:2478:A:C8   | 22:DA:2529:G:C5     | 2.92                     | 0.58              |
| 29:DH:108:VAL:O   | 29:DH:110:VAL:N     | 2.36                     | 0.58              |
| 36:DO:7:ARG:HD2   | 36:DO:97:PHE:CE1    | 2.38                     | 0.58              |
| 42:DU:41:LEU:HD12 | 42:DU:60:GLU:HG2    | 1.86                     | 0.58              |
| 1:AA:251:G:C6     | 1:AA:266:G:O6       | 2.56                     | 0.57              |
| 1:AA:673:A:H2'    | 1:AA:674:G:C8       | 2.39                     | 0.57              |
| 5:AE:109:GLY:O    | 5:AE:110:ALA:HB2    | 2.04                     | 0.57              |
| 22:BA:1922:G:H22  | 22:BA:1923:U:H1'    | 1.67                     | 0.57              |
| 22:BA:2190:G:C6   | 22:BA:2191:A:C5     | 2.91                     | 0.57              |
| 22:BA:2474:U:H5'' | 22:BA:2475:C:OP2    | 2.04                     | 0.57              |
| 22:BA:2520:C:C6   | 22:BA:2567:G:H1'    | 2.38                     | 0.57              |
| 22:BA:372:G:O2'   | 22:BA:400:G:O6      | 2.16                     | 0.57              |
| 22:BA:2531:A:OP2  | 28:BG:174:ALA:O     | 2.22                     | 0.57              |
| 30:BI:82:LYS:O    | 30:BI:83:ALA:HB2    | 2.04                     | 0.57              |
| 1:CA:1003:G:C2    | 1:CA:1038:C:C4      | 2.92                     | 0.57              |
| 1:CA:992:U:N3     | 1:CA:1043:G:N7      | 2.52                     | 0.57              |
| 4:CD:166:GLU:O    | 4:CD:167:LYS:HB2    | 2.04                     | 0.57              |
| 9:CI:30:ILE:HA    | 9:CI:65:ILE:O       | 2.03                     | 0.57              |
| 22:DA:1544:A:N6   | 22:DA:1545:A:N1     | 2.52                     | 0.57              |
| 22:DA:1774:C:O2   | 24:DC:11:PRO:HB2    | 2.04                     | 0.57              |
| 22:DA:776:G:O2'   | 22:DA:2241:A:OP1    | 2.19                     | 0.57              |
| 22:DA:2571:U:C4   | 22:DA:2574:G:C8     | 2.92                     | 0.57              |
| 22:DA:13:A:N1     | 22:DA:525:U:H2'     | 2.19                     | 0.57              |
| 22:DA:696:G:C2    | 22:DA:767:U:O2      | 2.57                     | 0.57              |
| 30:DI:79:LEU:HD13 | 30:DI:109:ILE:CG2   | 2.33                     | 0.57              |
| 35:DN:49:GLU:N    | 35:DN:50:PRO:CD     | 2.67                     | 0.57              |
| 1:AA:1157:A:N7    | 1:AA:1180:A:N6      | 2.51                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:AJ:92:LEU:O    | 10:AJ:93:ALA:CB   | 2.52                     | 0.57              |
| 53:B5:40:GLU:HA   | 53:B5:181:PHE:HA  | 1.85                     | 0.57              |
| 22:BA:1008:A:N6   | 22:BA:1136:G:C6   | 2.71                     | 0.57              |
| 22:BA:1061:U:O2'  | 22:BA:1062:G:C5'  | 2.52                     | 0.57              |
| 22:BA:742:A:H2'   | 22:BA:743:A:C8    | 2.39                     | 0.57              |
| 24:BC:125:LYS:HG2 | 24:BC:128:ASN:ND2 | 2.19                     | 0.57              |
| 29:BH:91:PHE:O    | 1:CA:55:A:C5      | 2.56                     | 0.57              |
| 22:BA:2009:A:OP1  | 40:BS:41:LYS:HE2  | 2.04                     | 0.57              |
| 1:CA:1093:A:C5    | 1:CA:1095:U:O4'   | 2.56                     | 0.57              |
| 1:CA:1224:U:C4    | 1:CA:1322:C:O2    | 2.56                     | 0.57              |
| 1:CA:1245:C:C4    | 1:CA:1246:A:N7    | 2.72                     | 0.57              |
| 2:CB:21:ARG:O     | 2:CB:23:TRP:N     | 2.37                     | 0.57              |
| 12:CL:38:TYR:CB   | 12:CL:52:VAL:HG13 | 2.34                     | 0.57              |
| 14:CN:54:ASP:HA   | 14:CN:59:ARG:HD3  | 1.86                     | 0.57              |
| 14:CN:91:GLY:O    | 14:CN:93:ILE:N    | 2.37                     | 0.57              |
| 17:CQ:50:ASN:O    | 17:CQ:52:GLU:N    | 2.37                     | 0.57              |
| 22:DA:1668:A:C4   | 22:DA:1674:G:N7   | 2.72                     | 0.57              |
| 22:DA:1965:C:OP1  | 22:DA:1966:A:H2'  | 2.03                     | 0.57              |
| 22:DA:2114:A:N6   | 22:DA:2119:A:N7   | 2.52                     | 0.57              |
| 22:DA:2293:G:H2'  | 22:DA:2294:G:O4'  | 2.04                     | 0.57              |
| 22:DA:2469:A:H4'  | 34:DM:55:ARG:HD3  | 1.84                     | 0.57              |
| 22:DA:247:G:C8    | 22:DA:249:C:C6    | 2.91                     | 0.57              |
| 22:DA:746:U:HO2'  | 22:DA:2611:C:HO2' | 1.50                     | 0.57              |
| 29:DH:62:LEU:C    | 29:DH:62:LEU:HD13 | 2.25                     | 0.57              |
| 33:DL:77:ILE:O    | 33:DL:110:VAL:O   | 2.21                     | 0.57              |
| 42:DU:13:VAL:HG21 | 42:DU:39:ILE:HD12 | 1.86                     | 0.57              |
| 22:DA:2387:U:H1'  | 44:DW:41:ARG:CD   | 2.34                     | 0.57              |
| 1:AA:208:U:C5     | 1:AA:210:C:N3     | 2.72                     | 0.57              |
| 4:AD:78:GLU:HG3   | 4:AD:93:LEU:HD21  | 1.86                     | 0.57              |
| 22:BA:1414:C:C4   | 22:BA:1415:U:C5   | 2.91                     | 0.57              |
| 24:BC:36:LYS:O    | 24:BC:37:ASN:CB   | 2.52                     | 0.57              |
| 35:BN:58:ASP:OD1  | 35:BN:63:ARG:NH2  | 2.37                     | 0.57              |
| 1:CA:1092:A:C6    | 1:CA:1183:U:O2    | 2.57                     | 0.57              |
| 1:CA:927:G:O2'    | 1:CA:1503:A:N7    | 2.31                     | 0.57              |
| 22:DA:1125:G:C6   | 22:DA:1126:A:N6   | 2.72                     | 0.57              |
| 22:DA:1827:U:C2'  | 22:DA:1828:G:O5'  | 2.52                     | 0.57              |
| 22:DA:1838:C:H4'  | 22:DA:1839:G:C8   | 2.39                     | 0.57              |
| 22:DA:2110:G:O2'  | 22:DA:2120:G:OP2  | 2.17                     | 0.57              |
| 22:DA:2267:A:H5'' | 22:DA:2268:A:H5'  | 1.85                     | 0.57              |
| 22:DA:2499:C:N4   | 22:DA:2500:U:O4   | 2.37                     | 0.57              |
| 22:DA:2537:U:H2'  | 22:DA:2538:C:C6   | 2.39                     | 0.57              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 22:DA:55:G:C2     | 22:DA:56:A:C8    | 2.92                     | 0.57              |
| 22:DA:740:C:C5'   | 22:DA:1784:A:H3' | 2.34                     | 0.57              |
| 23:DB:32:U:C2     | 23:DB:51:G:N2    | 2.72                     | 0.57              |
| 29:DH:117:LEU:HB3 | 29:DH:120:GLY:O  | 2.04                     | 0.57              |
| 1:AA:90:C:C2      | 1:AA:91:U:C6     | 2.92                     | 0.57              |
| 2:AB:222:ARG:CZ   | 2:AB:222:ARG:HB3 | 2.34                     | 0.57              |
| 4:AD:58:LYS:NZ    | 4:AD:69:GLU:OE2  | 2.33                     | 0.57              |
| 11:AK:52:PHE:CB   | 11:AK:56:ARG:HB3 | 2.35                     | 0.57              |
| 16:AP:75:ILE:HG22 | 16:AP:80:LYS:HE2 | 1.86                     | 0.57              |
| 22:BA:1179:G:C5   | 22:BA:1180:U:C1' | 2.86                     | 0.57              |
| 23:BB:48:U:H2'    | 23:BB:49:C:C6    | 2.39                     | 0.57              |
| 1:CA:1096:C:H2'   | 1:CA:1097:C:C6   | 2.39                     | 0.57              |
| 1:CA:1478:U:H2'   | 1:CA:1479:C:C6   | 2.39                     | 0.57              |
| 1:CA:206:C:H2'    | 1:CA:207:C:H5'   | 1.87                     | 0.57              |
| 1:CA:33:A:H2'     | 1:CA:34:C:C6     | 2.39                     | 0.57              |
| 4:CD:32:CYS:O     | 4:CD:33:LYS:CB   | 2.53                     | 0.57              |
| 8:CH:89:LYS:HA    | 8:CH:92:LEU:CD1  | 2.34                     | 0.57              |
| 22:DA:1344:U:O2'  | 22:DA:1345:C:P   | 2.63                     | 0.57              |
| 22:DA:1651:G:C2   | 22:DA:2007:U:O2  | 2.57                     | 0.57              |
| 22:DA:223:A:C4    | 22:DA:408:G:H1'  | 2.39                     | 0.57              |
| 22:DA:76:C:HO2'   | 46:DY:55:THR:HG1 | 1.51                     | 0.57              |
| 23:DB:81:G:C5     | 23:DB:82:U:C5    | 2.92                     | 0.57              |
| 24:DC:9:THR:O     | 24:DC:10:SER:CB  | 2.52                     | 0.57              |
| 39:DR:81:LYS:O    | 39:DR:82:HIS:C   | 2.42                     | 0.57              |
| 1:AA:144:G:C2     | 1:AA:179:A:N3    | 2.72                     | 0.57              |
| 1:AA:262:A:C6     | 1:AA:263:A:C6    | 2.93                     | 0.57              |
| 1:AA:299:G:H2'    | 1:AA:300:A:C8    | 2.40                     | 0.57              |
| 5:AE:13:GLU:CB    | 5:AE:39:VAL:HG12 | 2.34                     | 0.57              |
| 11:AK:51:GLY:O    | 11:AK:52:PHE:O   | 2.23                     | 0.57              |
| 22:BA:1079:C:C5   | 22:BA:1088:A:C2  | 2.93                     | 0.57              |
| 22:BA:1795:C:C4   | 22:BA:1796:U:C4  | 2.92                     | 0.57              |
| 22:BA:1958:C:O2'  | 22:BA:1959:G:H5' | 2.04                     | 0.57              |
| 22:BA:2615:U:C2   | 48:B0:4:GLN:HA   | 2.40                     | 0.57              |
| 22:BA:588:U:H2'   | 22:BA:589:U:C6   | 2.39                     | 0.57              |
| 22:BA:784:G:O2'   | 22:BA:785:G:H5'' | 2.04                     | 0.57              |
| 1:CA:455:G:N2     | 1:CA:478:A:C2    | 2.72                     | 0.57              |
| 1:CA:577:G:C4     | 1:CA:816:A:C2    | 2.92                     | 0.57              |
| 2:CB:210:VAL:O    | 2:CB:214:LEU:HB2 | 2.04                     | 0.57              |
| 7:CG:125:SER:O    | 7:CG:127:ALA:N   | 2.37                     | 0.57              |
| 9:CI:116:VAL:CG2  | 10:CJ:62:ARG:HD3 | 2.35                     | 0.57              |
| 22:DA:247:G:OP2   | 22:DA:249:C:N4   | 2.37                     | 0.57              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 22:DA:2612:C:H5''  | 22:DA:2613:U:OP1  | 2.05                     | 0.57              |
| 22:DA:411:G:OP1    | 57:DA:3558:HOH:O  | 2.17                     | 0.57              |
| 22:DA:616:A:C2     | 22:DA:617:G:O4'   | 2.57                     | 0.57              |
| 22:DA:634:C:H2'    | 22:DA:635:C:C6    | 2.40                     | 0.57              |
| 22:DA:674:G:H1'    | 26:DE:69:ARG:HE   | 1.69                     | 0.57              |
| 24:DC:31:ALA:N     | 24:DC:32:PRO:HD2  | 2.18                     | 0.57              |
| 24:DC:34:LEU:O     | 24:DC:35:GLU:HB3  | 2.03                     | 0.57              |
| 1:AA:1349:A:C2     | 1:AA:1374:A:C4    | 2.92                     | 0.57              |
| 1:AA:316:C:C2      | 1:AA:317:U:C5     | 2.92                     | 0.57              |
| 1:AA:32:A:C2       | 1:AA:33:A:C5      | 2.92                     | 0.57              |
| 1:AA:620:C:H2'     | 1:AA:621:A:O4'    | 2.04                     | 0.57              |
| 2:AB:147:SER:O     | 2:AB:148:LEU:HB2  | 2.04                     | 0.57              |
| 9:AI:57:MET:O      | 9:AI:59:GLU:N     | 2.38                     | 0.57              |
| 21:AU:10:GLU:CG    | 21:AU:11:PRO:HD3  | 2.35                     | 0.57              |
| 22:BA:1066:U:O2    | 22:BA:1069:A:N7   | 2.37                     | 0.57              |
| 22:BA:1712:U:OP2   | 22:BA:1713:A:O2'  | 2.20                     | 0.57              |
| 22:BA:2182:U:O4    | 22:BA:2183:A:N6   | 2.38                     | 0.57              |
| 24:BC:91:ILE:HD12  | 24:BC:103:TYR:CD1 | 2.40                     | 0.57              |
| 24:BC:141:VAL:HG11 | 24:BC:190:ALA:HB1 | 1.87                     | 0.57              |
| 43:BV:56:PHE:O     | 43:BV:61:LEU:HD11 | 2.04                     | 0.57              |
| 1:CA:145:G:C2      | 1:CA:146:G:C8     | 2.92                     | 0.57              |
| 1:CA:543:U:O2'     | 1:CA:544:G:H5'    | 2.03                     | 0.57              |
| 48:D0:55:ILE:O     | 48:D0:56:ALA:CB   | 2.53                     | 0.57              |
| 22:DA:1355:G:H2'   | 22:DA:1356:G:H5'  | 1.86                     | 0.57              |
| 22:DA:1446:C:H2'   | 22:DA:1447:C:O4'  | 2.04                     | 0.57              |
| 22:DA:1917:U:H2'   | 22:DA:1918:A:H5'  | 1.87                     | 0.57              |
| 22:DA:197:A:N6     | 22:DA:2430:A:H2'  | 2.18                     | 0.57              |
| 22:DA:2586:U:C5    | 22:DA:2587:A:C8   | 2.92                     | 0.57              |
| 1:AA:1154:G:C2     | 1:AA:1155:A:C5    | 2.92                     | 0.57              |
| 1:AA:1492:A:OP1    | 12:AL:44:LYS:N    | 2.37                     | 0.57              |
| 1:AA:65:A:C4       | 1:AA:381:C:C5     | 2.92                     | 0.57              |
| 1:AA:81:A:C2'      | 1:AA:82:G:H5''    | 2.35                     | 0.57              |
| 2:AB:184:PHE:CZ    | 2:AB:198:PHE:CD2  | 2.92                     | 0.57              |
| 5:AE:46:VAL:HG21   | 5:AE:118:ALA:HB2  | 1.87                     | 0.57              |
| 10:AJ:52:LEU:HB2   | 14:AN:81:ARG:NE   | 2.20                     | 0.57              |
| 17:AQ:48:ASP:C     | 17:AQ:48:ASP:OD2  | 2.43                     | 0.57              |
| 22:BA:1853:A:N1    | 22:BA:2087:G:H1'  | 2.19                     | 0.57              |
| 22:BA:482:A:H5''   | 22:BA:483:A:OP1   | 2.04                     | 0.57              |
| 22:BA:686:U:O4     | 50:B2:12:ARG:HB2  | 2.04                     | 0.57              |
| 22:BA:558:U:OP1    | 31:BJ:113:PRO:HD2 | 2.04                     | 0.57              |
| 32:BK:21:CYS:HA    | 32:BK:41:ILE:HG22 | 1.86                     | 0.57              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:CA:1178:G:N2    | 1:CA:1181:G:OP2    | 2.38                     | 0.57              |
| 1:CA:1302:C:C5    | 13:CM:17:ILE:HD13  | 2.40                     | 0.57              |
| 1:CA:1365:G:H2'   | 1:CA:1366:C:O4'    | 2.05                     | 0.57              |
| 2:CB:100:MET:HA   | 2:CB:107:VAL:HG21  | 1.87                     | 0.57              |
| 21:CU:10:GLU:HB2  | 21:CU:11:PRO:HD3   | 1.87                     | 0.57              |
| 22:DA:2888:C:H2'  | 22:DA:2889:C:C6    | 2.39                     | 0.57              |
| 22:DA:2504:U:C4   | 55:DA:3001:DOL:C16 | 2.88                     | 0.57              |
| 22:DA:498:G:C2    | 22:DA:499:U:C6     | 2.93                     | 0.57              |
| 22:DA:841:G:N2    | 22:DA:937:C:O2     | 2.33                     | 0.57              |
| 29:DH:21:VAL:HG22 | 29:DH:22:LYS:N     | 2.19                     | 0.57              |
| 22:DA:2360:G:H1'  | 33:DL:60:ARG:HD3   | 1.86                     | 0.57              |
| 35:DN:1:MET:CE    | 35:DN:1:MET:N      | 2.67                     | 0.57              |
| 1:AA:1107:C:N3    | 1:AA:1108:G:C8     | 2.73                     | 0.57              |
| 1:AA:19:A:N3      | 1:AA:917:G:C2      | 2.73                     | 0.57              |
| 1:AA:345:C:N3     | 32:BK:117:SER:OG   | 2.37                     | 0.57              |
| 1:AA:903:G:H2'    | 1:AA:904:U:H6      | 1.68                     | 0.57              |
| 2:AB:187:VAL:HG23 | 2:AB:187:VAL:O     | 2.04                     | 0.57              |
| 3:AC:64:ILE:HG23  | 3:AC:99:ALA:HB2    | 1.86                     | 0.57              |
| 5:AE:46:VAL:HG21  | 5:AE:118:ALA:CB    | 2.35                     | 0.57              |
| 10:AJ:53:ILE:CG2  | 10:AJ:61:ALA:HB1   | 2.35                     | 0.57              |
| 19:AS:5:LEU:HD23  | 19:AS:9:PRO:HA     | 1.87                     | 0.57              |
| 53:B5:125:GLY:O   | 53:B5:126:SER:CB   | 2.53                     | 0.57              |
| 53:B5:174:ALA:O   | 53:B5:175:PRO:CB   | 2.52                     | 0.57              |
| 22:BA:2897:U:H2'  | 22:BA:2898:U:C6    | 2.38                     | 0.57              |
| 29:BH:95:GLY:HA2  | 29:BH:117:LEU:HD22 | 1.87                     | 0.57              |
| 29:BH:132:PHE:CE2 | 29:BH:142:VAL:HG21 | 2.40                     | 0.57              |
| 31:BJ:81:ILE:HG23 | 31:BJ:82:GLY:H     | 1.69                     | 0.57              |
| 41:BT:17:SER:O    | 41:BT:20:ALA:N     | 2.37                     | 0.57              |
| 46:BY:18:LEU:O    | 46:BY:22:LEU:HB2   | 2.05                     | 0.57              |
| 4:CD:32:CYS:O     | 4:CD:33:LYS:HB3    | 2.05                     | 0.57              |
| 5:CE:154:ALA:HA   | 5:CE:157:ARG:HB3   | 1.86                     | 0.57              |
| 6:CF:86:ARG:HH11  | 6:CF:86:ARG:CG     | 2.17                     | 0.57              |
| 8:CH:96:MET:HB2   | 8:CH:99:LEU:O      | 2.03                     | 0.57              |
| 14:CN:80:SER:O    | 14:CN:82:ILE:N     | 2.37                     | 0.57              |
| 20:CT:28:MET:HE3  | 20:CT:58:VAL:HG22  | 1.87                     | 0.57              |
| 22:DA:2176:A:H2'  | 22:DA:2177:C:C6    | 2.39                     | 0.57              |
| 22:DA:2266:A:C2   | 22:DA:2272:U:C5    | 2.92                     | 0.57              |
| 22:DA:2697:G:C2   | 22:DA:2711:A:C2    | 2.92                     | 0.57              |
| 22:DA:324:A:N6    | 22:DA:338:G:O2'    | 2.37                     | 0.57              |
| 22:DA:67:U:C2     | 22:DA:68:G:C8      | 2.93                     | 0.57              |
| 22:DA:747:U:O4'   | 40:DS:92:ARG:NH1   | 2.37                     | 0.57              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:AA:1101:A:H4'    | 1:AA:1102:A:O5'   | 2.04                     | 0.57              |
| 1:AA:154:U:O2      | 1:AA:168:G:N2     | 2.37                     | 0.57              |
| 14:AN:51:LEU:CB    | 14:AN:52:PRO:HD2  | 2.34                     | 0.57              |
| 14:AN:52:PRO:O     | 14:AN:53:ARG:HB3  | 2.04                     | 0.57              |
| 1:AA:1313:U:P      | 19:AS:6:LYS:HB3   | 2.45                     | 0.57              |
| 22:BA:1378:A:C4    | 22:BA:1380:G:N7   | 2.73                     | 0.57              |
| 22:BA:2582:G:C2    | 22:BA:2583:G:C8   | 2.92                     | 0.57              |
| 22:BA:304:U:H2'    | 22:BA:305:C:C6    | 2.40                     | 0.57              |
| 24:BC:15:HIS:O     | 24:BC:204:VAL:CG2 | 2.52                     | 0.57              |
| 28:BG:87:LEU:N     | 28:BG:87:LEU:HD12 | 2.20                     | 0.57              |
| 29:BH:117:LEU:HD21 | 29:BH:121:VAL:CA  | 2.35                     | 0.57              |
| 29:BH:117:LEU:CD2  | 29:BH:121:VAL:H   | 2.08                     | 0.57              |
| 38:BQ:87:SER:HB3   | 39:BR:51:VAL:HA   | 1.87                     | 0.57              |
| 1:CA:60:A:N3       | 1:CA:61:G:H1'     | 2.20                     | 0.57              |
| 1:CA:636:U:H2'     | 1:CA:637:C:C6     | 2.39                     | 0.57              |
| 1:CA:992:U:C4      | 1:CA:1043:G:N7    | 2.73                     | 0.57              |
| 2:CB:210:VAL:HG22  | 2:CB:211:THR:N    | 2.18                     | 0.57              |
| 5:CE:104:GLY:O     | 5:CE:105:ILE:CG2  | 2.53                     | 0.57              |
| 5:CE:24:THR:HA     | 5:CE:29:ARG:HA    | 1.86                     | 0.57              |
| 12:CL:80:ILE:HD12  | 12:CL:97:THR:HG21 | 1.87                     | 0.57              |
| 16:CP:51:ARG:C     | 16:CP:51:ARG:HD3  | 2.25                     | 0.57              |
| 16:CP:38:PHE:CE2   | 16:CP:51:ARG:HD2  | 2.40                     | 0.57              |
| 20:CT:25:ARG:HD2   | 20:CT:29:ARG:NH1  | 2.19                     | 0.57              |
| 22:DA:1826:G:C6    | 22:DA:1827:U:C4   | 2.92                     | 0.57              |
| 22:DA:2148:G:C2    | 22:DA:2149:U:C5   | 2.93                     | 0.57              |
| 22:DA:2308:G:C5'   | 22:DA:2309:A:OP2  | 2.51                     | 0.57              |
| 22:DA:249:C:P      | 22:DA:2394:C:HO2' | 2.27                     | 0.57              |
| 30:DI:10:LYS:HB2   | 30:DI:56:PRO:CB   | 2.34                     | 0.57              |
| 36:DO:33:ARG:O     | 36:DO:34:HIS:CB   | 2.52                     | 0.57              |
| 22:DA:2019:A:H4'   | 38:DQ:34:VAL:CG2  | 2.35                     | 0.57              |
| 1:AA:502:A:H2'     | 1:AA:503:C:O4'    | 2.05                     | 0.57              |
| 5:AE:25:VAL:O      | 5:AE:26:LYS:C     | 2.43                     | 0.57              |
| 22:BA:253:C:OP2    | 51:B3:5:LYS:CE    | 2.53                     | 0.57              |
| 53:B5:180:SER:CB   | 53:B5:188:ASP:CB  | 2.83                     | 0.57              |
| 53:B5:51:ASP:N     | 53:B5:52:PRO:HD3  | 2.20                     | 0.57              |
| 22:BA:2153:C:H2'   | 22:BA:2154:A:O4'  | 2.05                     | 0.57              |
| 22:BA:70:G:H4'     | 22:BA:71:A:OP1    | 2.04                     | 0.57              |
| 22:BA:877:A:N6     | 22:BA:899:A:N6    | 2.53                     | 0.57              |
| 22:BA:2485:G:OP1   | 34:BM:45:GLN:NE2  | 2.37                     | 0.57              |
| 4:CD:173:VAL:O     | 4:CD:174:ASP:HB3  | 2.05                     | 0.57              |
| 7:CG:92:ARG:HB3    | 7:CG:93:PRO:HD2   | 1.86                     | 0.57              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 19:CS:55:ARG:CZ   | 19:CS:79:THR:HG22 | 2.34                     | 0.57              |
| 22:DA:106:C:HO2'  | 22:DA:294:A:HO2'  | 0.58                     | 0.57              |
| 22:DA:1313:U:H2'  | 22:DA:1313:U:O2   | 2.05                     | 0.57              |
| 22:DA:1651:G:N2   | 22:DA:2007:U:O2   | 2.38                     | 0.57              |
| 22:DA:235:U:C4    | 22:DA:236:C:C5    | 2.92                     | 0.57              |
| 22:DA:2707:U:H2'  | 22:DA:2708:G:C8   | 2.39                     | 0.57              |
| 22:DA:445:C:O2'   | 22:DA:449:A:N3    | 2.37                     | 0.57              |
| 22:DA:1570:A:H5'  | 24:DC:36:LYS:HB3  | 1.85                     | 0.57              |
| 22:DA:807:U:OP2   | 33:DL:41:ARG:NH1  | 2.37                     | 0.57              |
| 1:AA:582:C:C4     | 1:AA:583:A:N7     | 2.73                     | 0.56              |
| 9:AI:47:VAL:HA    | 9:AI:50:GLN:HB2   | 1.87                     | 0.56              |
| 1:CA:575:G:C6     | 1:CA:821:G:N7     | 2.73                     | 0.56              |
| 2:CB:184:PHE:CE1  | 2:CB:198:PHE:CD2  | 2.93                     | 0.56              |
| 5:CE:98:PRO:O     | 5:CE:122:ASN:ND2  | 2.33                     | 0.56              |
| 6:CF:45:ARG:HD2   | 6:CF:59:TYR:CE2   | 2.40                     | 0.56              |
| 8:CH:126:ILE:HD12 | 8:CH:126:ILE:N    | 2.20                     | 0.56              |
| 9:CI:32:GLN:NE2   | 9:CI:64:TYR:OH    | 2.38                     | 0.56              |
| 15:CO:62:GLN:O    | 15:CO:66:LEU:HD23 | 2.05                     | 0.56              |
| 22:DA:2429:G:N7   | 33:DL:55:MET:HE3  | 2.19                     | 0.56              |
| 22:DA:88:G:C2     | 22:DA:89:A:C8     | 2.93                     | 0.56              |
| 32:DK:104:THR:O   | 32:DK:106:GLU:N   | 2.38                     | 0.56              |
| 40:DS:29:VAL:CG1  | 40:DS:55:ILE:HD11 | 2.35                     | 0.56              |
| 42:DU:34:VAL:HG23 | 42:DU:65:ILE:O    | 2.04                     | 0.56              |
| 1:AA:1520:C:C2    | 1:AA:1521:C:C5    | 2.93                     | 0.56              |
| 1:AA:832:G:C2     | 1:AA:833:G:C8     | 2.93                     | 0.56              |
| 2:AB:67:ILE:HG21  | 2:AB:69:PHE:CE2   | 2.40                     | 0.56              |
| 2:AB:88:ASP:C     | 2:AB:89:GLN:HG3   | 2.25                     | 0.56              |
| 20:AT:71:LYS:HD2  | 20:AT:74:ARG:NH2  | 2.20                     | 0.56              |
| 22:BA:1436:G:N2   | 22:BA:1557:C:C2   | 2.73                     | 0.56              |
| 22:BA:2394:C:OP2  | 51:B3:30:ARG:HD3  | 2.04                     | 0.56              |
| 22:BA:578:G:OP1   | 22:BA:1255:U:O2'  | 2.22                     | 0.56              |
| 40:BS:62:ASP:O    | 40:BS:63:GLY:O    | 2.23                     | 0.56              |
| 2:CB:83:ALA:O     | 2:CB:86:SER:OG    | 2.22                     | 0.56              |
| 12:CL:107:VAL:CG2 | 12:CL:117:TYR:HB3 | 2.35                     | 0.56              |
| 22:DA:1068:G:N3   | 22:DA:1068:G:H2'  | 2.19                     | 0.56              |
| 22:DA:1530:G:C2   | 22:DA:1542:U:O2   | 2.58                     | 0.56              |
| 22:DA:1683:U:O5'  | 22:DA:1683:U:H6   | 1.87                     | 0.56              |
| 22:DA:1826:G:C5   | 22:DA:1827:U:C5   | 2.93                     | 0.56              |
| 25:DD:176:ASP:HB2 | 25:DD:190:LYS:HB3 | 1.87                     | 0.56              |
| 31:DJ:41:LYS:O    | 31:DJ:42:ALA:C    | 2.44                     | 0.56              |
| 33:DL:94:THR:O    | 33:DL:98:ALA:N    | 2.37                     | 0.56              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:AA:429:U:H1'   | 1:AA:430:A:H5''   | 1.88                     | 0.56              |
| 3:AC:12:LEU:O    | 3:AC:13:GLY:C     | 2.44                     | 0.56              |
| 7:AG:99:LEU:O    | 7:AG:101:MET:N    | 2.38                     | 0.56              |
| 21:AU:44:GLU:OE2 | 21:AU:45:ARG:NH1  | 2.38                     | 0.56              |
| 22:BA:1324:G:C4  | 22:BA:1328:A:N6   | 2.73                     | 0.56              |
| 22:BA:1808:A:N1  | 45:BX:28:ARG:HD2  | 2.21                     | 0.56              |
| 22:BA:1901:A:OP2 | 24:BC:253:LYS:NZ  | 2.33                     | 0.56              |
| 22:BA:1922:G:N2  | 22:BA:1923:U:C1'  | 2.68                     | 0.56              |
| 22:BA:45:G:H5''  | 22:BA:46:G:H5'    | 1.87                     | 0.56              |
| 22:BA:967:U:H2'  | 22:BA:968:C:C6    | 2.40                     | 0.56              |
| 23:BB:110:C:C4   | 23:BB:111:U:C5    | 2.94                     | 0.56              |
| 30:BI:18:ALA:C   | 30:BI:20:PRO:HD3  | 2.26                     | 0.56              |
| 34:BM:51:ARG:O   | 34:BM:55:ARG:HG3  | 2.05                     | 0.56              |
| 1:CA:1394:A:C5   | 1:CA:1501:C:H4'   | 2.40                     | 0.56              |
| 1:CA:411:A:C6    | 1:CA:429:U:C5     | 2.93                     | 0.56              |
| 1:CA:562:U:OP2   | 12:CL:14:ARG:NE   | 2.38                     | 0.56              |
| 5:CE:96:MET:HE3  | 5:CE:111:MET:CE   | 2.34                     | 0.56              |
| 15:CO:37:ASN:O   | 15:CO:40:GLN:CB   | 2.52                     | 0.56              |
| 52:D4:36:ARG:HG2 | 52:D4:37:GLN:N    | 2.20                     | 0.56              |
| 22:DA:1410:G:C2  | 22:DA:1411:U:C4   | 2.93                     | 0.56              |
| 22:DA:783:A:O2'  | 22:DA:1779:U:O2   | 2.14                     | 0.56              |
| 22:DA:491:G:C6   | 22:DA:492:A:C6    | 2.93                     | 0.56              |
| 22:DA:971:G:H2'  | 22:DA:972:A:O4'   | 2.04                     | 0.56              |
| 28:DG:86:LYS:HB3 | 28:DG:165:ALA:HB2 | 1.87                     | 0.56              |
| 22:DA:2757:A:N1  | 28:DG:67:THR:HG21 | 2.20                     | 0.56              |
| 1:AA:1367:C:OP2  | 9:AI:114:LYS:NZ   | 2.37                     | 0.56              |
| 1:AA:604:G:C2    | 1:AA:635:A:C2     | 2.93                     | 0.56              |
| 5:AE:157:ARG:C   | 5:AE:159:LYS:N    | 2.58                     | 0.56              |
| 10:AJ:34:ALA:O   | 10:AJ:35:GLN:CB   | 2.52                     | 0.56              |
| 20:AT:44:LYS:CD  | 20:AT:87:ALA:HA   | 2.36                     | 0.56              |
| 48:B0:15:MET:O   | 48:B0:18:SER:CB   | 2.53                     | 0.56              |
| 22:BA:1352:U:O2' | 22:BA:1353:A:H5'  | 2.05                     | 0.56              |
| 22:BA:1926:U:O2  | 22:BA:1928:A:N7   | 2.38                     | 0.56              |
| 22:BA:894:U:H2'  | 22:BA:895:U:C6    | 2.39                     | 0.56              |
| 27:BF:123:ASP:CG | 27:BF:127:ASN:HB2 | 2.26                     | 0.56              |
| 1:CA:1330:U:H4'  | 13:CM:23:TYR:CE1  | 2.39                     | 0.56              |
| 3:CC:77:ILE:HA   | 3:CC:84:VAL:CG2   | 2.35                     | 0.56              |
| 12:CL:44:LYS:CB  | 12:CL:45:PRO:CD   | 2.83                     | 0.56              |
| 13:CM:91:HIS:CD2 | 13:CM:97:VAL:HG21 | 2.40                     | 0.56              |
| 22:DA:1353:A:C8  | 22:DA:1378:A:N6   | 2.73                     | 0.56              |
| 22:DA:2093:G:O2' | 22:DA:2094:A:H5'  | 2.04                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:DA:457:A:N1    | 22:DA:470:A:H5''  | 2.20                     | 0.56              |
| 22:DA:64:A:H2'    | 22:DA:65:U:O4'    | 2.05                     | 0.56              |
| 22:DA:1844:C:O3'  | 24:DC:256:LYS:NZ  | 2.38                     | 0.56              |
| 22:DA:2310:C:C4   | 27:DF:77:PHE:CZ   | 2.94                     | 0.56              |
| 22:DA:2379:G:H4'  | 36:DO:21:LEU:HD11 | 1.87                     | 0.56              |
| 37:DP:93:ARG:O    | 37:DP:94:LYS:CB   | 2.54                     | 0.56              |
| 41:DT:21:SER:O    | 41:DT:22:THR:C    | 2.43                     | 0.56              |
| 41:DT:89:GLU:O    | 41:DT:91:GLN:N    | 2.38                     | 0.56              |
| 1:AA:1135:U:C2'   | 1:AA:1136:C:O5'   | 2.54                     | 0.56              |
| 1:AA:1068:G:O2'   | 1:AA:1191:A:N1    | 2.24                     | 0.56              |
| 2:AB:186:ILE:HA   | 2:AB:200:ILE:O    | 2.06                     | 0.56              |
| 22:BA:1073:A:C3'  | 22:BA:1074:G:H5'' | 2.35                     | 0.56              |
| 22:BA:878:A:N6    | 22:BA:899:A:O2'   | 2.36                     | 0.56              |
| 23:BB:34:A:O2'    | 23:BB:35:C:H5''   | 2.05                     | 0.56              |
| 37:BP:31:TRP:CE2  | 37:BP:40:LEU:CD1  | 2.88                     | 0.56              |
| 39:BR:51:VAL:HG23 | 39:BR:52:PRO:HD2  | 1.87                     | 0.56              |
| 1:CA:991:U:C4     | 1:CA:1212:U:O4'   | 2.58                     | 0.56              |
| 1:CA:922:G:H4'    | 5:CE:25:VAL:HA    | 1.88                     | 0.56              |
| 1:CA:972:C:H4'    | 10:CJ:59:LYS:HG2  | 1.88                     | 0.56              |
| 21:CU:35:ARG:NH2  | 57:CU:101:HOH:O   | 2.38                     | 0.56              |
| 22:DA:1181:U:H2'  | 22:DA:1182:G:C8   | 2.40                     | 0.56              |
| 22:DA:1817:G:C2'  | 22:DA:1818:U:H5'  | 2.36                     | 0.56              |
| 22:DA:1973:G:C6   | 22:DA:1974:C:N4   | 2.73                     | 0.56              |
| 22:DA:2189:U:H2'  | 22:DA:2190:G:H5'  | 1.87                     | 0.56              |
| 22:DA:2341:G:C6   | 22:DA:2342:C:C4   | 2.94                     | 0.56              |
| 22:DA:749:A:C4    | 22:DA:750:A:C8    | 2.94                     | 0.56              |
| 29:DH:83:LYS:N    | 29:DH:149:GLU:HG2 | 2.20                     | 0.56              |
| 1:AA:1289:A:O3'   | 7:AG:35:LYS:NZ    | 2.37                     | 0.56              |
| 1:AA:631:C:C5'    | 1:AA:632:U:O5'    | 2.54                     | 0.56              |
| 1:AA:880:C:O2'    | 1:AA:881:G:H5'    | 2.06                     | 0.56              |
| 9:AI:57:MET:CG    | 9:AI:58:VAL:H     | 2.18                     | 0.56              |
| 13:AM:95:LEU:HB3  | 13:AM:96:PRO:HD2  | 1.87                     | 0.56              |
| 18:AR:34:THR:OG1  | 18:AR:35:GLU:N    | 2.38                     | 0.56              |
| 20:AT:54:MET:HE1  | 20:AT:58:VAL:HG21 | 1.87                     | 0.56              |
| 48:B0:55:ILE:HG22 | 48:B0:57:LYS:H    | 1.70                     | 0.56              |
| 22:BA:2191:A:N1   | 22:BA:2192:U:O4   | 2.39                     | 0.56              |
| 30:BI:82:LYS:O    | 30:BI:83:ALA:CB   | 2.53                     | 0.56              |
| 40:BS:57:ASN:O    | 40:BS:61:ASN:HB2  | 2.04                     | 0.56              |
| 1:CA:106:C:C2'    | 1:CA:107:G:H5'    | 2.35                     | 0.56              |
| 1:CA:1224:U:N3    | 1:CA:1322:C:O2    | 2.38                     | 0.56              |
| 1:CA:169:C:H2'    | 1:CA:170:U:C6     | 2.40                     | 0.56              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:CA:32:A:H2'     | 1:CA:32:A:N3       | 2.20                     | 0.56              |
| 8:CH:64:LYS:HB3   | 8:CH:71:VAL:HG21   | 1.87                     | 0.56              |
| 22:DA:1986:C:OP1  | 57:DA:3429:HOH:O   | 2.18                     | 0.56              |
| 22:DA:858:G:C4    | 22:DA:2268:A:C2    | 2.94                     | 0.56              |
| 22:DA:2845:U:H2'  | 22:DA:2846:G:O4'   | 2.05                     | 0.56              |
| 22:DA:983:A:N6    | 22:DA:984:A:C2     | 2.73                     | 0.56              |
| 1:AA:375:U:C4     | 1:AA:376:G:N7      | 2.74                     | 0.56              |
| 1:AA:71:A:O2'     | 1:AA:72:A:P        | 2.62                     | 0.56              |
| 10:AJ:43:PRO:O    | 10:AJ:71:LEU:HD23  | 2.06                     | 0.56              |
| 22:BA:2502:G:C5'  | 22:BA:2503:A:H5''  | 2.36                     | 0.56              |
| 22:BA:2680:U:O2'  | 22:BA:2681:C:H5'   | 2.05                     | 0.56              |
| 34:BM:70:ASP:OD2  | 34:BM:70:ASP:C     | 2.44                     | 0.56              |
| 1:CA:1262:C:C4    | 1:CA:1263:C:C4     | 2.94                     | 0.56              |
| 1:CA:802:A:N3     | 1:CA:802:A:H2'     | 2.21                     | 0.56              |
| 2:CB:143:LYS:O    | 2:CB:147:SER:OG    | 2.19                     | 0.56              |
| 3:CC:61:ALA:O     | 3:CC:62:LYS:HB2    | 2.05                     | 0.56              |
| 4:CD:62:ARG:NH1   | 4:CD:69:GLU:OE1    | 2.38                     | 0.56              |
| 4:CD:70:ARG:O     | 4:CD:74:ASN:ND2    | 2.39                     | 0.56              |
| 5:CE:34:THR:HB    | 5:CE:50:TYR:CZ     | 2.41                     | 0.56              |
| 5:CE:98:PRO:O     | 5:CE:99:ALA:HB3    | 2.05                     | 0.56              |
| 8:CH:21:ASN:O     | 8:CH:22:LYS:C      | 2.42                     | 0.56              |
| 9:CI:55:VAL:CG2   | 9:CI:55:VAL:O      | 2.53                     | 0.56              |
| 11:CK:25:ALA:HB3  | 11:CK:87:LYS:O     | 2.05                     | 0.56              |
| 16:CP:70:ARG:O    | 16:CP:74:LEU:HD23  | 2.05                     | 0.56              |
| 22:DA:12:U:O2     | 22:DA:12:U:H2'     | 2.06                     | 0.56              |
| 22:DA:1581:G:C5   | 22:DA:1582:C:C4    | 2.94                     | 0.56              |
| 22:DA:2325:G:C6   | 22:DA:2326:C:N4    | 2.73                     | 0.56              |
| 22:DA:295:G:H2'   | 22:DA:295:G:N3     | 2.20                     | 0.56              |
| 22:DA:571:U:C4    | 22:DA:575:A:C5     | 2.94                     | 0.56              |
| 22:DA:696:G:N1    | 22:DA:767:U:C2     | 2.73                     | 0.56              |
| 22:DA:936:A:C2    | 22:DA:937:C:C2     | 2.94                     | 0.56              |
| 24:DC:18:LYS:O    | 24:DC:19:VAL:HB    | 2.04                     | 0.56              |
| 28:DG:118:PRO:HG3 | 28:DG:144:VAL:HG21 | 1.87                     | 0.56              |
| 38:DQ:50:ARG:O    | 38:DQ:54:LYS:NZ    | 2.36                     | 0.56              |
| 5:AE:109:GLY:O    | 5:AE:110:ALA:CB    | 2.52                     | 0.56              |
| 13:AM:4:ILE:O     | 13:AM:6:GLY:N      | 2.39                     | 0.56              |
| 22:BA:1073:A:C3'  | 22:BA:1074:G:C5'   | 2.80                     | 0.56              |
| 22:BA:1180:U:C2'  | 22:BA:1181:U:H5'   | 2.36                     | 0.56              |
| 22:BA:137:U:H2'   | 22:BA:140:C:C2     | 2.41                     | 0.56              |
| 22:BA:1680:U:H2'  | 22:BA:1681:G:O4'   | 2.06                     | 0.56              |
| 22:BA:2888:C:O2   | 22:BA:2888:C:H2'   | 2.06                     | 0.56              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:BA:523:C:O2'    | 22:BA:524:G:H5'    | 2.06                     | 0.56              |
| 22:BA:563:A:C2     | 22:BA:564:C:C2     | 2.94                     | 0.56              |
| 22:BA:77:G:N2      | 22:BA:110:G:H1'    | 2.21                     | 0.56              |
| 29:BH:40:THR:OG1   | 29:BH:43:ASN:OD1   | 2.24                     | 0.56              |
| 36:BO:41:ALA:HB2   | 36:BO:48:LEU:HD21  | 1.88                     | 0.56              |
| 40:BS:8:ARG:O      | 40:BS:9:HIS:HB2    | 2.06                     | 0.56              |
| 43:BV:6:ALA:HB1    | 43:BV:40:ILE:HG23  | 1.88                     | 0.56              |
| 46:BY:34:SER:O     | 46:BY:36:GLN:N     | 2.39                     | 0.56              |
| 1:CA:1069:C:C2'    | 1:CA:1070:U:O5'    | 2.54                     | 0.56              |
| 3:CC:130:PHE:CZ    | 3:CC:131:ARG:HD2   | 2.41                     | 0.56              |
| 12:CL:90:LEU:HB3   | 12:CL:93:VAL:CG2   | 2.36                     | 0.56              |
| 21:CU:47:ARG:HE    | 21:CU:47:ARG:HA    | 1.70                     | 0.56              |
| 22:DA:1310:G:C2'   | 22:DA:1311:G:H5'   | 2.35                     | 0.56              |
| 22:DA:2216:G:H2'   | 22:DA:2217:G:C8    | 2.40                     | 0.56              |
| 22:DA:629:G:N3     | 22:DA:639:U:O2'    | 2.37                     | 0.56              |
| 22:DA:686:U:H2'    | 22:DA:788:A:N1     | 2.21                     | 0.56              |
| 26:DE:149:ILE:HG12 | 26:DE:188:MET:SD   | 2.45                     | 0.56              |
| 26:DE:196:VAL:O    | 26:DE:196:VAL:HG12 | 2.04                     | 0.56              |
| 30:DI:101:ILE:O    | 30:DI:102:SER:HB3  | 2.05                     | 0.56              |
| 34:DM:72:PRO:HB3   | 34:DM:92:TRP:CZ3   | 2.40                     | 0.56              |
| 39:DR:52:PRO:O     | 39:DR:53:PHE:CB    | 2.53                     | 0.56              |
| 1:AA:542:G:OP1     | 4:AD:10:LYS:CE     | 2.54                     | 0.56              |
| 1:AA:821:G:H4'     | 57:AA:1741:HOH:O   | 2.05                     | 0.56              |
| 5:AE:157:ARG:HD2   | 8:AH:43:GLU:O      | 2.05                     | 0.56              |
| 8:AH:95:VAL:HG12   | 8:AH:96:MET:N      | 2.20                     | 0.56              |
| 10:AJ:27:GLU:C     | 10:AJ:29:ALA:H     | 2.10                     | 0.56              |
| 17:AQ:45:HIS:CG    | 17:AQ:70:THR:CG2   | 2.88                     | 0.56              |
| 22:BA:2120:G:N2    | 22:BA:2179:C:O2    | 2.39                     | 0.56              |
| 22:BA:2820:A:C6    | 25:BD:197:THR:CG2  | 2.88                     | 0.56              |
| 22:BA:936:A:H2'    | 22:BA:937:C:C6     | 2.41                     | 0.56              |
| 23:BB:30:C:OP1     | 36:BO:3:LYS:NZ     | 2.39                     | 0.56              |
| 43:BV:58:SER:O     | 43:BV:73:LYS:HE2   | 2.06                     | 0.56              |
| 1:CA:1069:C:H2'    | 1:CA:1070:U:O5'    | 2.06                     | 0.56              |
| 1:CA:1190:G:H5'    | 3:CC:176:HIS:CE1   | 2.41                     | 0.56              |
| 1:CA:1394:A:N1     | 1:CA:1500:A:O2'    | 2.36                     | 0.56              |
| 1:CA:182:A:C5      | 1:CA:184:G:N7      | 2.74                     | 0.56              |
| 1:CA:577:G:N9      | 1:CA:816:A:C2      | 2.74                     | 0.56              |
| 1:CA:635:A:C6      | 1:CA:636:U:C4      | 2.93                     | 0.56              |
| 2:CB:54:LEU:HA     | 2:CB:57:LEU:HB3    | 1.86                     | 0.56              |
| 4:CD:168:PRO:CB    | 4:CD:171:LEU:HD12  | 2.36                     | 0.56              |
| 1:CA:426:U:H5''    | 4:CD:37:ALA:HB1    | 1.87                     | 0.56              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 11:CK:84:VAL:HG11  | 11:CK:97:ILE:HG22  | 1.88                     | 0.56              |
| 16:CP:16:PHE:CE1   | 16:CP:38:PHE:HB2   | 2.41                     | 0.56              |
| 22:DA:126:A:N7     | 22:DA:127:A:N1     | 2.53                     | 0.56              |
| 22:DA:1315:C:O2'   | 22:DA:1392:A:N3    | 2.36                     | 0.56              |
| 22:DA:1638:C:H4'   | 22:DA:2710:C:O2    | 2.05                     | 0.56              |
| 22:DA:491:G:C6     | 22:DA:492:A:C5     | 2.93                     | 0.56              |
| 22:DA:1843:C:H4'   | 24:DC:251:GLN:CD   | 2.25                     | 0.56              |
| 32:DK:31:ARG:HB3   | 32:DK:32:TYR:CE2   | 2.41                     | 0.56              |
| 35:DN:54:LEU:HD21  | 35:DN:66:ALA:HB2   | 1.87                     | 0.56              |
| 1:AA:1109:C:OP2    | 3:AC:176:HIS:ND1   | 2.32                     | 0.56              |
| 1:AA:11:G:C6       | 1:AA:12:U:C4       | 2.94                     | 0.56              |
| 1:AA:205:A:H2'     | 1:AA:205:A:N3      | 2.21                     | 0.56              |
| 1:AA:527:G:O2'     | 1:AA:535:A:N1      | 2.36                     | 0.56              |
| 1:AA:57:G:H2'      | 1:AA:58:C:C6       | 2.41                     | 0.56              |
| 1:AA:858:G:O6      | 1:AA:869:G:C8      | 2.58                     | 0.56              |
| 4:AD:37:ALA:HA     | 4:AD:42:GLY:HA3    | 1.87                     | 0.56              |
| 6:AF:91:ARG:HG3    | 6:AF:92:THR:N      | 2.19                     | 0.56              |
| 22:BA:1565:C:OP1   | 24:BC:18:LYS:NZ    | 2.39                     | 0.56              |
| 22:BA:1838:C:C6    | 22:BA:1899:A:C6    | 2.94                     | 0.56              |
| 22:BA:572:A:C2     | 22:BA:2033:A:C2    | 2.94                     | 0.56              |
| 24:BC:86:ASN:N     | 24:BC:86:ASN:OD1   | 2.37                     | 0.56              |
| 25:BD:103:ASP:O    | 25:BD:104:VAL:HG22 | 2.06                     | 0.56              |
| 32:BK:106:GLU:OE2  | 32:BK:106:GLU:N    | 2.38                     | 0.56              |
| 46:BY:9:LYS:O      | 46:BY:12:GLU:N     | 2.38                     | 0.56              |
| 1:CA:496:A:C2      | 1:CA:497:G:C6      | 2.93                     | 0.56              |
| 1:CA:502:A:H2'     | 1:CA:503:C:O4'     | 2.06                     | 0.56              |
| 2:CB:10:LEU:CD2    | 2:CB:12:ALA:O      | 2.54                     | 0.56              |
| 2:CB:15:HIS:O      | 2:CB:15:HIS:CG     | 2.58                     | 0.56              |
| 2:CB:162:PHE:HA    | 2:CB:184:PHE:O     | 2.06                     | 0.56              |
| 3:CC:75:ILE:O      | 3:CC:75:ILE:HG13   | 2.05                     | 0.56              |
| 5:CE:125:ALA:O     | 5:CE:126:LYS:HB3   | 2.05                     | 0.56              |
| 49:D1:21:TYR:CD1   | 49:D1:38:LYS:HD2   | 2.41                     | 0.56              |
| 22:DA:1153:C:H5'   | 38:DQ:62:ILE:HD13  | 1.87                     | 0.56              |
| 22:DA:1351:C:H2'   | 22:DA:1352:U:O4'   | 2.06                     | 0.56              |
| 22:DA:1973:G:C5    | 22:DA:1974:C:C5    | 2.94                     | 0.56              |
| 22:DA:2262:U:H1'   | 22:DA:2328:A:H1'   | 1.87                     | 0.56              |
| 31:DJ:105:VAL:HG12 | 31:DJ:109:LEU:HD12 | 1.88                     | 0.56              |
| 47:DZ:40:ASP:OD2   | 47:DZ:45:ARG:NH1   | 2.38                     | 0.56              |
| 1:AA:452:A:H2'     | 1:AA:453:G:C5'     | 2.36                     | 0.56              |
| 4:AD:32:CYS:O      | 4:AD:33:LYS:CB     | 2.54                     | 0.56              |
| 15:AO:19:ALA:O     | 15:AO:20:ASN:HB2   | 2.06                     | 0.56              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:BA:1115:G:N3   | 22:BA:1116:G:C8   | 2.73                     | 0.56              |
| 22:BA:2286:G:O6   | 49:B1:23:THR:OG1  | 2.10                     | 0.56              |
| 37:BP:40:LEU:HD21 | 37:BP:82:ASP:OD2  | 2.06                     | 0.56              |
| 46:BY:9:LYS:HB3   | 46:BY:12:GLU:HG3  | 1.87                     | 0.56              |
| 1:CA:898:G:N2     | 1:CA:901:A:OP2    | 2.36                     | 0.56              |
| 2:CB:219:ALA:O    | 2:CB:220:THR:HB   | 2.05                     | 0.56              |
| 12:CL:82:ILE:HD11 | 12:CL:95:TYR:HB2  | 1.88                     | 0.56              |
| 22:DA:1355:G:C2'  | 22:DA:1356:G:H5'  | 2.36                     | 0.56              |
| 22:DA:1440:U:H2'  | 22:DA:1441:G:O4'  | 2.06                     | 0.56              |
| 22:DA:927:A:O2'   | 47:DZ:39:GLU:OE1  | 2.23                     | 0.56              |
| 45:DX:31:PRO:HB2  | 45:DX:33:LEU:CD1  | 2.36                     | 0.56              |
| 1:AA:764:C:H5''   | 15:AO:50:HIS:CD2  | 2.40                     | 0.55              |
| 17:AQ:16:LYS:C    | 17:AQ:17:MET:HE3  | 2.26                     | 0.55              |
| 49:B1:7:GLU:OE1   | 49:B1:53:LYS:O    | 2.24                     | 0.55              |
| 51:B3:27:ALA:O    | 51:B3:28:ASN:CB   | 2.53                     | 0.55              |
| 22:BA:1179:G:C5   | 22:BA:1180:U:N1   | 2.74                     | 0.55              |
| 22:BA:1422:G:C4   | 22:BA:1423:G:C8   | 2.94                     | 0.55              |
| 22:BA:2492:U:C2   | 22:BA:2493:U:C5   | 2.93                     | 0.55              |
| 36:BO:25:ARG:HG3  | 36:BO:27:VAL:HG12 | 1.88                     | 0.55              |
| 36:BO:31:THR:HG22 | 36:BO:34:HIS:N    | 2.20                     | 0.55              |
| 38:BQ:9:ILE:O     | 38:BQ:13:ARG:HG3  | 2.07                     | 0.55              |
| 1:CA:1255:G:N1    | 1:CA:1279:G:C8    | 2.74                     | 0.55              |
| 3:CC:74:GLY:O     | 3:CC:78:GLY:N     | 2.39                     | 0.55              |
| 4:CD:107:PHE:CG   | 4:CD:145:ILE:HD11 | 2.41                     | 0.55              |
| 20:CT:67:ILE:HD12 | 20:CT:71:LYS:HE3  | 1.87                     | 0.55              |
| 21:CU:37:PHE:HA   | 21:CU:40:LYS:HE3  | 1.87                     | 0.55              |
| 22:DA:948:C:O2    | 22:DA:984:A:O2'   | 2.21                     | 0.55              |
| 44:DW:49:ALA:O    | 44:DW:50:ASN:HB2  | 2.06                     | 0.55              |
| 1:AA:108:G:C5'    | 1:AA:108:G:N3     | 2.70                     | 0.55              |
| 1:AA:1287:A:H2'   | 1:AA:1288:A:C8    | 2.41                     | 0.55              |
| 1:AA:554:A:H2'    | 1:AA:555:U:C6     | 2.41                     | 0.55              |
| 1:AA:782:A:C2     | 1:AA:801:U:C2     | 2.95                     | 0.55              |
| 2:AB:93:ASN:OD1   | 2:AB:94:HIS:ND1   | 2.38                     | 0.55              |
| 3:AC:145:GLY:O    | 3:AC:146:ALA:C    | 2.44                     | 0.55              |
| 5:AE:151:GLU:O    | 5:AE:153:VAL:N    | 2.38                     | 0.55              |
| 6:AF:3:HIS:H      | 6:AF:92:THR:HG23  | 1.71                     | 0.55              |
| 9:AI:9:THR:HG22   | 9:AI:10:GLY:N     | 2.21                     | 0.55              |
| 22:BA:1181:U:H2'  | 22:BA:1182:G:C8   | 2.41                     | 0.55              |
| 22:BA:1327:A:N6   | 22:BA:1328:A:C2   | 2.74                     | 0.55              |
| 22:BA:1385:A:C4   | 22:BA:1386:C:C5   | 2.95                     | 0.55              |
| 22:BA:1832:C:C4   | 22:BA:1833:C:C5   | 2.94                     | 0.55              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 22:BA:1857:G:N2    | 22:BA:1884:G:H1'    | 2.20                     | 0.55              |
| 22:BA:511:U:C5     | 22:BA:512:G:C5      | 2.95                     | 0.55              |
| 22:BA:574:A:OP2    | 57:BA:3267:HOH:O    | 2.18                     | 0.55              |
| 22:BA:588:U:H1'    | 26:BE:85:PHE:CD1    | 2.41                     | 0.55              |
| 22:BA:84:A:H4'     | 22:BA:85:G:O5'      | 2.06                     | 0.55              |
| 27:BF:108:VAL:HG13 | 27:BF:114:PHE:CE2   | 2.42                     | 0.55              |
| 32:BK:109:SER:O    | 32:BK:110:GLU:C     | 2.44                     | 0.55              |
| 40:BS:30:SER:OG    | 40:BS:31:GLN:N      | 2.36                     | 0.55              |
| 43:BV:32:GLY:O     | 43:BV:93:ARG:NH1    | 2.38                     | 0.55              |
| 1:CA:1041:G:H2'    | 1:CA:1042:A:C8      | 2.40                     | 0.55              |
| 1:CA:109:A:C6      | 1:CA:327:A:C6       | 2.94                     | 0.55              |
| 1:CA:1296:C:H4'    | 1:CA:1302:C:N4      | 2.21                     | 0.55              |
| 1:CA:1439:G:C2     | 1:CA:1463:U:O2      | 2.59                     | 0.55              |
| 4:CD:160:GLU:O     | 4:CD:163:GLU:HB2    | 2.06                     | 0.55              |
| 22:DA:1034:G:C6    | 22:DA:1035:U:N3     | 2.74                     | 0.55              |
| 22:DA:1179:G:C5    | 22:DA:1180:U:H1'    | 2.41                     | 0.55              |
| 22:DA:770:G:H1'    | 22:DA:1379:U:C4     | 2.41                     | 0.55              |
| 22:DA:1754:A:C6    | 22:DA:1755:A:C6     | 2.94                     | 0.55              |
| 22:DA:2202:U:H5''  | 22:DA:2203:U:OP1    | 2.06                     | 0.55              |
| 22:DA:269:C:O2     | 22:DA:269:C:H2'     | 2.06                     | 0.55              |
| 22:DA:2725:A:C4    | 22:DA:2727:A:C8     | 2.93                     | 0.55              |
| 55:DA:3001:DOL:N9  | 55:DA:3001:DOL:HC41 | 2.21                     | 0.55              |
| 22:DA:319:G:C4     | 22:DA:333:G:N2      | 2.75                     | 0.55              |
| 22:DA:694:U:H2'    | 22:DA:695:G:H5''    | 1.87                     | 0.55              |
| 22:DA:842:U:N3     | 22:DA:843:G:N7      | 2.54                     | 0.55              |
| 25:DD:151:THR:HG22 | 25:DD:152:PRO:N     | 2.22                     | 0.55              |
| 36:DO:100:HIS:CD2  | 36:DO:101:GLY:N     | 2.75                     | 0.55              |
| 1:AA:1064:G:O2'    | 1:AA:1190:G:N2      | 2.39                     | 0.55              |
| 2:AB:24:ASN:O      | 2:AB:26:LYS:N       | 2.40                     | 0.55              |
| 5:AE:97:GLN:HB3    | 5:AE:124:LEU:HD12   | 1.87                     | 0.55              |
| 6:AF:98:GLU:CG     | 6:AF:99:ALA:N       | 2.69                     | 0.55              |
| 53:B5:19:LYS:HG3   | 53:B5:23:ILE:CG1    | 2.37                     | 0.55              |
| 22:BA:1916:A:C2    | 22:BA:1917:U:O2     | 2.59                     | 0.55              |
| 22:BA:422:A:N1     | 22:BA:423:A:C2      | 2.74                     | 0.55              |
| 23:BB:15:A:O2'     | 23:BB:16:G:H5'      | 2.06                     | 0.55              |
| 22:BA:2845:U:H5''  | 37:BP:52:ASN:O      | 2.04                     | 0.55              |
| 1:CA:466:A:C2      | 1:CA:468:A:C8       | 2.95                     | 0.55              |
| 1:CA:798:U:H2'     | 1:CA:799:G:O5'      | 2.07                     | 0.55              |
| 8:CH:18:GLN:NE2    | 8:CH:70:ALA:HB1     | 2.21                     | 0.55              |
| 52:D4:36:ARG:CG    | 52:D4:37:GLN:N      | 2.68                     | 0.55              |
| 22:DA:1562:U:H2'   | 22:DA:1563:U:O4'    | 2.07                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:DA:2112:G:N3   | 22:DA:2112:G:H2'  | 2.22                     | 0.55              |
| 22:DA:2805:C:H2'  | 22:DA:2806:C:C6   | 2.40                     | 0.55              |
| 22:DA:2815:C:H2'  | 22:DA:2816:G:C8   | 2.42                     | 0.55              |
| 31:DJ:36:LEU:O    | 31:DJ:121:LYS:NZ  | 2.39                     | 0.55              |
| 1:AA:1236:A:H2'   | 1:AA:1237:C:C6    | 2.40                     | 0.55              |
| 1:AA:1387:G:H2'   | 1:AA:1388:C:C6    | 2.41                     | 0.55              |
| 1:AA:872:A:C8     | 1:AA:874:G:C8     | 2.95                     | 0.55              |
| 2:AB:49:MET:O     | 2:AB:53:ALA:HB2   | 2.05                     | 0.55              |
| 11:AK:25:ALA:HA   | 11:AK:30:THR:HG22 | 1.87                     | 0.55              |
| 22:BA:142:A:C5    | 22:BA:143:C:N4    | 2.75                     | 0.55              |
| 22:BA:1688:U:N3   | 22:BA:1698:A:C2   | 2.75                     | 0.55              |
| 22:BA:1731:G:C6   | 22:BA:1733:G:C5   | 2.94                     | 0.55              |
| 22:BA:528:A:H3'   | 22:BA:528:A:H8    | 1.71                     | 0.55              |
| 22:BA:580:U:H2'   | 22:BA:581:C:C6    | 2.41                     | 0.55              |
| 25:BD:71:ALA:HB1  | 25:BD:92:VAL:HG13 | 1.87                     | 0.55              |
| 31:BJ:60:ASP:HA   | 31:BJ:97:PRO:HB3  | 1.89                     | 0.55              |
| 22:BA:1199:U:H1'  | 38:BQ:4:VAL:HG22  | 1.89                     | 0.55              |
| 41:BT:2:ILE:HA    | 41:BT:3:ARG:HB2   | 1.88                     | 0.55              |
| 1:CA:1012:A:C2    | 1:CA:1018:G:C2    | 2.94                     | 0.55              |
| 1:CA:1071:C:H2'   | 1:CA:1072:G:H8    | 1.71                     | 0.55              |
| 1:CA:734:G:C4     | 1:CA:735:C:C5     | 2.94                     | 0.55              |
| 4:CD:161:LEU:HD23 | 4:CD:162:ALA:N    | 2.21                     | 0.55              |
| 9:CI:25:ASN:O     | 9:CI:27:LYS:N     | 2.39                     | 0.55              |
| 22:DA:1360:G:O6   | 22:DA:1372:U:C2   | 2.60                     | 0.55              |
| 22:DA:1532:A:C2   | 22:DA:1540:G:C6   | 2.93                     | 0.55              |
| 22:DA:1767:G:O6   | 22:DA:1986:C:N4   | 2.39                     | 0.55              |
| 22:DA:1826:G:O2'  | 22:DA:1971:U:OP2  | 2.23                     | 0.55              |
| 22:DA:526:A:C6    | 22:DA:2626:C:H4'  | 2.41                     | 0.55              |
| 22:DA:2718:G:C6   | 22:DA:2719:G:C4   | 2.94                     | 0.55              |
| 22:DA:406:G:H2'   | 22:DA:407:G:O4'   | 2.06                     | 0.55              |
| 22:DA:449:A:C5    | 22:DA:450:G:C8    | 2.94                     | 0.55              |
| 22:DA:584:C:N4    | 22:DA:585:G:C6    | 2.75                     | 0.55              |
| 23:DB:39:A:H2'    | 23:DB:40:U:C6     | 2.41                     | 0.55              |
| 30:DI:80:LEU:HA   | 30:DI:84:ALA:CB   | 2.35                     | 0.55              |
| 41:DT:12:ARG:O    | 41:DT:13:ALA:HB2  | 2.05                     | 0.55              |
| 1:AA:1441:A:H2'   | 1:AA:1442:G:O5'   | 2.05                     | 0.55              |
| 1:AA:340:U:H2'    | 1:AA:341:C:C6     | 2.42                     | 0.55              |
| 1:AA:403:C:OP1    | 4:AD:134:SER:OG   | 2.18                     | 0.55              |
| 1:AA:781:A:H4'    | 1:AA:1522:U:O2'   | 2.06                     | 0.55              |
| 2:AB:53:ALA:O     | 2:AB:57:LEU:HB2   | 2.06                     | 0.55              |
| 4:AD:103:TYR:HB2  | 4:AD:114:ALA:CB   | 2.36                     | 0.55              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 53:B5:56:ASP:OD2  | 53:B5:58:ASN:ND2  | 2.40                     | 0.55              |
| 22:BA:1176:U:C4   | 22:BA:1177:G:O6   | 2.60                     | 0.55              |
| 22:BA:1494:A:O2'  | 22:BA:1495:A:O5'  | 2.24                     | 0.55              |
| 22:BA:973:A:H5'   | 22:BA:1188:U:H1'  | 1.88                     | 0.55              |
| 27:BF:175:PHE:HD1 | 27:BF:177:PHE:CE1 | 2.25                     | 0.55              |
| 36:BO:29:HIS:CD2  | 36:BO:29:HIS:C    | 2.79                     | 0.55              |
| 44:BW:23:VAL:HA   | 44:BW:38:VAL:HG12 | 1.89                     | 0.55              |
| 1:CA:328:C:O2     | 1:CA:328:C:C2'    | 2.54                     | 0.55              |
| 1:CA:427:U:O2'    | 1:CA:541:G:OP1    | 2.17                     | 0.55              |
| 29:BH:91:PHE:CD1  | 1:CA:55:A:C8      | 2.94                     | 0.55              |
| 3:CC:134:MET:SD   | 3:CC:153:VAL:CG1  | 2.95                     | 0.55              |
| 4:CD:107:PHE:O    | 4:CD:117:LEU:HD11 | 2.07                     | 0.55              |
| 9:CI:19:VAL:HG21  | 9:CI:82:GLY:CA    | 2.36                     | 0.55              |
| 22:DA:1360:G:N1   | 22:DA:1361:G:H1'  | 2.22                     | 0.55              |
| 22:DA:1810:A:H5'' | 22:DA:1811:G:OP2  | 2.05                     | 0.55              |
| 22:DA:2420:C:OP1  | 51:D3:34:THR:HB   | 2.06                     | 0.55              |
| 22:DA:1801:A:C5   | 24:DC:262:ARG:NH2 | 2.75                     | 0.55              |
| 25:DD:16:THR:OG1  | 25:DD:18:ASP:OD2  | 2.12                     | 0.55              |
| 31:DJ:39:LYS:HZ3  | 31:DJ:39:LYS:HB2  | 1.72                     | 0.55              |
| 36:DO:33:ARG:O    | 36:DO:34:HIS:HB2  | 2.06                     | 0.55              |
| 22:DA:483:A:C2    | 42:DU:58:ILE:HD11 | 2.41                     | 0.55              |
| 1:AA:1419:G:C5    | 1:AA:1420:U:C5    | 2.95                     | 0.55              |
| 1:AA:320:A:H2'    | 1:AA:321:A:C1'    | 2.36                     | 0.55              |
| 4:AD:152:GLN:O    | 4:AD:153:SER:C    | 2.44                     | 0.55              |
| 4:AD:91:LEU:HD11  | 4:AD:195:ILE:HD11 | 1.89                     | 0.55              |
| 6:AF:17:GLN:OE1   | 6:AF:24:ARG:NH2   | 2.39                     | 0.55              |
| 7:AG:120:LEU:HD13 | 7:AG:124:LEU:HD23 | 1.88                     | 0.55              |
| 9:AI:114:LYS:HG2  | 9:AI:120:LYS:HA   | 1.86                     | 0.55              |
| 9:AI:6:TYR:HB3    | 9:AI:89:GLU:HG2   | 1.87                     | 0.55              |
| 12:AL:56:ARG:NH1  | 12:AL:62:GLU:HG3  | 2.21                     | 0.55              |
| 18:AR:25:ASP:O    | 18:AR:27:ALA:N    | 2.39                     | 0.55              |
| 22:BA:1915:U:C2   | 22:BA:1916:A:C8   | 2.94                     | 0.55              |
| 22:BA:1268:A:C2   | 22:BA:2013:A:C4   | 2.94                     | 0.55              |
| 22:BA:2286:G:H5'' | 22:BA:2287:A:O4'  | 2.06                     | 0.55              |
| 22:BA:2318:G:C5   | 22:BA:2319:G:C6   | 2.95                     | 0.55              |
| 22:BA:2820:A:C2'  | 22:BA:2821:A:OP1  | 2.55                     | 0.55              |
| 22:BA:528:A:N1    | 22:BA:2043:C:H5'  | 2.22                     | 0.55              |
| 27:BF:85:ILE:O    | 27:BF:85:ILE:CG1  | 2.55                     | 0.55              |
| 29:BH:86:ASP:O    | 29:BH:87:GLU:CB   | 2.53                     | 0.55              |
| 29:BH:98:ASP:O    | 29:BH:102:ALA:HB3 | 2.07                     | 0.55              |
| 42:BU:13:VAL:HG12 | 42:BU:19:LYS:HA   | 1.88                     | 0.55              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:CA:1000:A:C2     | 1:CA:1041:G:N2    | 2.74                     | 0.55              |
| 1:CA:1255:G:C6     | 1:CA:1279:G:N7    | 2.74                     | 0.55              |
| 1:CA:1288:A:N1     | 1:CA:1371:G:H1'   | 2.21                     | 0.55              |
| 1:CA:137:U:H1'     | 1:CA:227:G:N2     | 2.21                     | 0.55              |
| 5:CE:90:THR:HG22   | 5:CE:91:GLY:N     | 2.21                     | 0.55              |
| 22:DA:1323:C:C4    | 22:DA:1324:G:N7   | 2.74                     | 0.55              |
| 22:DA:749:A:C5     | 22:DA:1618:A:C2   | 2.95                     | 0.55              |
| 22:DA:1645:G:OP1   | 22:DA:1646:C:H5'  | 2.06                     | 0.55              |
| 22:DA:2353:G:H2'   | 22:DA:2354:C:O4'  | 2.06                     | 0.55              |
| 26:DE:108:ILE:HD11 | 26:DE:180:LEU:HB2 | 1.87                     | 0.55              |
| 28:DG:176:LYS:O    | 28:DG:177:LYS:CB  | 2.54                     | 0.55              |
| 33:DL:55:MET:SD    | 33:DL:59:ARG:NH2  | 2.80                     | 0.55              |
| 33:DL:81:ASP:O     | 33:DL:82:LEU:HB3  | 2.05                     | 0.55              |
| 22:DA:484:C:OP1    | 42:DU:48:PRO:HG3  | 2.07                     | 0.55              |
| 46:DY:27:ASN:HA    | 46:DY:30:MET:HB2  | 1.89                     | 0.55              |
| 22:DA:95:A:O2'     | 46:DY:40:SER:N    | 2.39                     | 0.55              |
| 1:AA:1144:G:H5''   | 1:AA:1145:A:OP2   | 2.07                     | 0.55              |
| 1:AA:1418:A:C2     | 1:AA:1483:A:C2    | 2.94                     | 0.55              |
| 1:AA:957:U:H1'     | 1:AA:960:U:N3     | 2.22                     | 0.55              |
| 3:AC:11:ARG:NH1    | 3:AC:182:ILE:HB   | 2.22                     | 0.55              |
| 3:AC:155:GLY:HA2   | 3:AC:163:ALA:HB1  | 1.88                     | 0.55              |
| 5:AE:81:LEU:HA     | 5:AE:147:MET:HE1  | 1.88                     | 0.55              |
| 11:AK:30:THR:HG21  | 11:AK:91:PRO:O    | 2.06                     | 0.55              |
| 22:BA:1789:A:OP2   | 24:BC:221:ARG:NH1 | 2.40                     | 0.55              |
| 1:CA:1007:U:C4     | 1:CA:1008:U:C5    | 2.95                     | 0.55              |
| 1:CA:1107:C:C4     | 1:CA:1108:G:N7    | 2.75                     | 0.55              |
| 1:CA:1363:A:O2'    | 1:CA:1365:G:N7    | 2.36                     | 0.55              |
| 1:CA:1491:G:C6     | 1:CA:1492:A:N1    | 2.75                     | 0.55              |
| 9:CI:12:ARG:CZ     | 9:CI:107:ASP:OD2  | 2.53                     | 0.55              |
| 1:CA:718:A:H5'     | 11:CK:119:ASN:CG  | 2.27                     | 0.55              |
| 19:CS:80:TYR:O     | 19:CS:81:ARG:CB   | 2.54                     | 0.55              |
| 50:D2:18:PHE:O     | 50:D2:21:ARG:N    | 2.40                     | 0.55              |
| 22:DA:1510:G:H2'   | 22:DA:1511:G:O4'  | 2.06                     | 0.55              |
| 22:DA:1606:C:C2'   | 22:DA:1607:C:OP2  | 2.55                     | 0.55              |
| 22:DA:1917:U:C2'   | 22:DA:1918:A:H5'  | 2.37                     | 0.55              |
| 22:DA:2395:C:H2'   | 22:DA:2396:G:O4'  | 2.06                     | 0.55              |
| 22:DA:669:G:C2     | 22:DA:801:G:N1    | 2.74                     | 0.55              |
| 1:AA:92:U:H2'      | 1:AA:93:U:C6      | 2.41                     | 0.55              |
| 22:BA:1949:G:N2    | 22:BA:1958:C:O2   | 2.40                     | 0.55              |
| 22:BA:1959:G:H2'   | 22:BA:1960:A:O5'  | 2.07                     | 0.55              |
| 22:BA:2580:U:C5    | 22:BA:2581:G:C6   | 2.94                     | 0.55              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 22:BA:350:G:H2'    | 22:BA:351:C:O4'   | 2.06                     | 0.55              |
| 29:BH:121:VAL:N    | 29:BH:122:LEU:CA  | 2.69                     | 0.55              |
| 29:BH:120:GLY:CA   | 29:BH:122:LEU:HA  | 2.37                     | 0.55              |
| 39:BR:49:ILE:C     | 39:BR:51:VAL:O    | 2.45                     | 0.55              |
| 1:CA:1521:C:C2     | 1:CA:1522:U:C6    | 2.94                     | 0.55              |
| 1:CA:786:G:N2      | 1:CA:787:A:H1'    | 2.22                     | 0.55              |
| 1:CA:840:C:N3      | 1:CA:842:U:H4'    | 2.22                     | 0.55              |
| 1:CA:909:A:H2'     | 1:CA:910:C:O4'    | 2.07                     | 0.55              |
| 22:DA:1020:A:C2    | 22:DA:1141:U:C2   | 2.95                     | 0.55              |
| 22:DA:1395:A:O2'   | 22:DA:1397:U:C6   | 2.59                     | 0.55              |
| 22:DA:187:G:N2     | 22:DA:210:C:H1'   | 2.22                     | 0.55              |
| 22:DA:320:A:H4'    | 22:DA:322:A:C8    | 2.42                     | 0.55              |
| 22:DA:667:U:C4     | 22:DA:668:A:N7    | 2.75                     | 0.55              |
| 22:DA:753:A:C2     | 22:DA:754:U:C2    | 2.94                     | 0.55              |
| 25:DD:151:THR:HG22 | 25:DD:152:PRO:CD  | 2.37                     | 0.55              |
| 29:DH:31:VAL:HB    | 29:DH:32:PRO:HD3  | 1.89                     | 0.55              |
| 46:DY:31:GLN:HG2   | 46:DY:36:GLN:HB2  | 1.89                     | 0.55              |
| 1:AA:1138:G:C2     | 1:AA:1140:C:C5    | 2.94                     | 0.55              |
| 1:AA:1462:C:H2'    | 1:AA:1463:U:O4'   | 2.06                     | 0.55              |
| 1:AA:1464:U:OP2    | 37:BP:109:ARG:NH1 | 2.40                     | 0.55              |
| 1:AA:451:A:H61     | 1:AA:481:G:H5'    | 1.72                     | 0.55              |
| 1:AA:66:A:C6       | 1:AA:67:C:C5      | 2.95                     | 0.55              |
| 1:AA:89:U:O2'      | 1:AA:90:C:H5'     | 2.07                     | 0.55              |
| 1:AA:995:C:N3      | 1:AA:1046:A:O2'   | 2.36                     | 0.55              |
| 4:AD:195:ILE:HG13  | 4:AD:195:ILE:O    | 2.04                     | 0.55              |
| 12:AL:94:ARG:HB2   | 12:AL:95:TYR:CE2  | 2.42                     | 0.55              |
| 13:AM:37:ALA:CB    | 13:AM:56:LEU:HD23 | 2.37                     | 0.55              |
| 20:AT:28:MET:O     | 20:AT:32:ILE:HG13 | 2.06                     | 0.55              |
| 22:BA:1080:A:H2'   | 22:BA:1080:A:N3   | 2.22                     | 0.55              |
| 22:BA:1309:G:H4'   | 50:B2:7:PRO:HB2   | 1.88                     | 0.55              |
| 22:BA:1355:G:O2'   | 22:BA:1356:G:H5'  | 2.07                     | 0.55              |
| 22:BA:1494:A:H2'   | 22:BA:1495:A:O5'  | 2.06                     | 0.55              |
| 22:BA:1668:A:H4'   | 22:BA:1669:A:O5'  | 2.07                     | 0.55              |
| 22:BA:2480:C:C2'   | 22:BA:2481:G:H5'  | 2.37                     | 0.55              |
| 22:BA:2765:A:N3    | 22:BA:2765:A:H2'  | 2.22                     | 0.55              |
| 22:BA:78:U:H2'     | 22:BA:79:C:C6     | 2.42                     | 0.55              |
| 29:BH:121:VAL:N    | 29:BH:122:LEU:CB  | 2.70                     | 0.55              |
| 22:BA:2846:G:OP2   | 37:BP:52:ASN:HB2  | 2.07                     | 0.55              |
| 2:CB:141:LEU:O     | 2:CB:145:GLU:N    | 2.37                     | 0.55              |
| 6:CF:18:VAL:HG12   | 6:CF:19:PRO:N     | 2.22                     | 0.55              |
| 6:CF:97:THR:O      | 6:CF:98:GLU:CB    | 2.55                     | 0.55              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 8:CH:2:SER:C       | 8:CH:4:GLN:N        | 2.60                     | 0.55              |
| 12:CL:90:LEU:CB    | 12:CL:93:VAL:HG21   | 2.37                     | 0.55              |
| 22:DA:1060:U:H4'   | 22:DA:1061:U:H5'    | 1.89                     | 0.55              |
| 22:DA:1127:A:H2'   | 22:DA:1128:G:H5''   | 1.89                     | 0.55              |
| 22:DA:1992:G:N2    | 22:DA:1996:C:O2'    | 2.39                     | 0.55              |
| 22:DA:2307:G:N2    | 22:DA:2312:U:N3     | 2.55                     | 0.55              |
| 22:DA:411:G:OP2    | 22:DA:2406:A:O2'    | 2.20                     | 0.55              |
| 22:DA:419:U:C4     | 22:DA:420:C:C5      | 2.95                     | 0.55              |
| 22:DA:672:C:C2     | 22:DA:809:G:N2      | 2.75                     | 0.55              |
| 22:DA:1808:A:N1    | 45:DX:28:ARG:HD2    | 2.21                     | 0.55              |
| 45:DX:43:GLU:O     | 45:DX:44:LYS:C      | 2.44                     | 0.55              |
| 1:AA:144:G:C5      | 1:AA:179:A:C2       | 2.95                     | 0.55              |
| 1:AA:66:A:H4'      | 1:AA:173:U:C5       | 2.42                     | 0.55              |
| 4:AD:152:GLN:O     | 4:AD:155:VAL:HG12   | 2.06                     | 0.55              |
| 13:AM:16:VAL:HG22  | 13:AM:41:GLU:HB2    | 1.88                     | 0.55              |
| 22:BA:26:G:H1'     | 22:BA:514:A:N6      | 2.22                     | 0.55              |
| 35:BN:79:LEU:O     | 35:BN:80:PHE:HB2    | 2.06                     | 0.55              |
| 1:CA:106:C:H2'     | 1:CA:107:G:H5'      | 1.89                     | 0.55              |
| 1:CA:769:G:H4'     | 1:CA:1513:A:H4'     | 1.88                     | 0.55              |
| 1:CA:280:C:N3      | 17:CQ:40:ARG:HA     | 2.22                     | 0.55              |
| 1:CA:31:G:O4'      | 1:CA:306:A:C2       | 2.60                     | 0.55              |
| 3:CC:172:ARG:HG3   | 3:CC:174:PRO:HD3    | 1.89                     | 0.55              |
| 21:CU:8:GLU:HB3    | 21:CU:12:PHE:CE2    | 2.42                     | 0.55              |
| 51:D3:4:ILE:HG21   | 51:D3:63:PRO:HG3    | 1.89                     | 0.55              |
| 22:DA:1318:U:H2'   | 22:DA:1319:C:C6     | 2.42                     | 0.55              |
| 22:DA:2107:G:C2    | 22:DA:2183:A:C2     | 2.95                     | 0.55              |
| 22:DA:2261:C:C2    | 22:DA:2280:G:C2     | 2.95                     | 0.55              |
| 22:DA:315:G:H2'    | 22:DA:316:C:O4'     | 2.06                     | 0.55              |
| 22:DA:420:C:H2'    | 22:DA:421:C:C6      | 2.42                     | 0.55              |
| 24:DC:141:VAL:HG11 | 24:DC:190:ALA:HB1   | 1.88                     | 0.55              |
| 25:DD:125:TRP:CE3  | 25:DD:160:LYS:HD3   | 2.42                     | 0.55              |
| 23:DB:52:A:C4      | 36:DO:33:ARG:NH2    | 2.75                     | 0.55              |
| 5:AE:149:SER:CB    | 5:AE:152:MET:HB2    | 2.37                     | 0.54              |
| 5:AE:81:LEU:HB3    | 5:AE:147:MET:CE     | 2.36                     | 0.54              |
| 12:AL:72:HIS:ND1   | 12:AL:72:HIS:O      | 2.40                     | 0.54              |
| 22:BA:1965:C:OP1   | 22:BA:1966:A:O2'    | 2.07                     | 0.54              |
| 22:BA:2196:C:C2'   | 22:BA:2197:U:H5'    | 2.36                     | 0.54              |
| 22:BA:2415:G:H2'   | 22:BA:2416:C:C6     | 2.42                     | 0.54              |
| 22:BA:2694:G:H2'   | 22:BA:2695:U:C6     | 2.42                     | 0.54              |
| 22:BA:2506:U:C4    | 55:BA:3001:DOL:H422 | 2.41                     | 0.54              |
| 22:BA:55:G:C2      | 22:BA:56:A:C8       | 2.95                     | 0.54              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 29:BH:10:ALA:O    | 29:BH:12:LEU:N     | 2.40                     | 0.54              |
| 30:BI:16:GLY:HA2  | 30:BI:51:LYS:HB3   | 1.89                     | 0.54              |
| 38:BQ:110:VAL:O   | 38:BQ:114:LYS:HG3  | 2.07                     | 0.54              |
| 1:CA:1072:G:C5    | 1:CA:1073:U:C5     | 2.95                     | 0.54              |
| 1:CA:1240:U:C5    | 7:CG:109:ARG:NH1   | 2.76                     | 0.54              |
| 1:CA:466:A:N1     | 1:CA:468:A:N7      | 2.55                     | 0.54              |
| 1:CA:53:A:C2      | 1:CA:359:G:C6      | 2.95                     | 0.54              |
| 1:CA:939:G:C6     | 1:CA:940:C:N4      | 2.75                     | 0.54              |
| 1:CA:97:G:C5      | 1:CA:98:A:H1'      | 2.42                     | 0.54              |
| 5:CE:36:LEU:HD21  | 5:CE:137:VAL:HG11  | 1.89                     | 0.54              |
| 12:CL:3:THR:HB    | 12:CL:6:GLN:HG3    | 1.89                     | 0.54              |
| 12:CL:83:ARG:CG   | 12:CL:84:GLY:N     | 2.70                     | 0.54              |
| 12:CL:88:LYS:O    | 12:CL:88:LYS:HG3   | 2.07                     | 0.54              |
| 15:CO:27:VAL:HG12 | 15:CO:28:GLN:N     | 2.21                     | 0.54              |
| 22:DA:1027:A:N7   | 22:DA:1126:A:C2    | 2.74                     | 0.54              |
| 22:DA:1352:U:C5   | 22:DA:1377:G:C6    | 2.95                     | 0.54              |
| 22:DA:565:C:H4'   | 22:DA:1253:A:N6    | 2.23                     | 0.54              |
| 22:DA:630:G:H3'   | 22:DA:631:A:C5'    | 2.37                     | 0.54              |
| 22:DA:732:C:H2'   | 22:DA:733:G:O4'    | 2.06                     | 0.54              |
| 22:DA:581:C:OP2   | 38:DQ:33:ARG:CZ    | 2.54                     | 0.54              |
| 42:DU:96:PHE:CZ   | 42:DU:103:ILE:HG13 | 2.41                     | 0.54              |
| 42:DU:54:GLN:N    | 42:DU:55:PRO:CD    | 2.70                     | 0.54              |
| 1:AA:266:G:H4'    | 1:AA:267:C:OP1     | 2.06                     | 0.54              |
| 1:AA:91:U:H2'     | 1:AA:92:U:O4'      | 2.08                     | 0.54              |
| 6:AF:84:VAL:O     | 6:AF:84:VAL:HG22   | 2.07                     | 0.54              |
| 22:BA:2517:C:C6   | 22:BA:2542:A:N7    | 2.75                     | 0.54              |
| 29:BH:90:LEU:CD2  | 29:BH:93:SER:HA    | 2.37                     | 0.54              |
| 39:BR:49:ILE:CG2  | 39:BR:52:PRO:C     | 2.76                     | 0.54              |
| 47:BZ:14:ILE:HG22 | 47:BZ:15:GLY:N     | 2.21                     | 0.54              |
| 1:CA:577:G:H1'    | 1:CA:816:A:N3      | 2.23                     | 0.54              |
| 1:CA:801:U:C2     | 1:CA:802:A:N7      | 2.75                     | 0.54              |
| 2:CB:53:ALA:O     | 2:CB:57:LEU:HB2    | 2.07                     | 0.54              |
| 4:CD:22:LYS:O     | 4:CD:23:SER:C      | 2.45                     | 0.54              |
| 1:CA:614:C:OP1    | 4:CD:83:LYS:NZ     | 2.39                     | 0.54              |
| 9:CI:54:LEU:O     | 9:CI:55:VAL:HG22   | 2.08                     | 0.54              |
| 22:DA:1096:A:C5   | 22:DA:1097:U:C5    | 2.95                     | 0.54              |
| 22:DA:1131:G:OP1  | 31:DJ:82:GLY:HA2   | 2.07                     | 0.54              |
| 22:DA:277:G:C2'   | 22:DA:361:G:O6     | 2.55                     | 0.54              |
| 22:DA:569:U:H5''  | 22:DA:821:A:C2     | 2.43                     | 0.54              |
| 22:DA:919:U:H2'   | 22:DA:920:A:O4'    | 2.07                     | 0.54              |
| 23:DB:78:A:C5     | 23:DB:99:A:C8      | 2.96                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 24:DC:92:ALA:HB3   | 24:DC:104:ILE:CD1  | 2.37                     | 0.54              |
| 26:DE:108:ILE:HD11 | 26:DE:180:LEU:CB   | 2.37                     | 0.54              |
| 29:DH:79:THR:HA    | 29:DH:145:ASN:HB2  | 1.89                     | 0.54              |
| 42:DU:44:LYS:HE3   | 42:DU:46:GLN:HB2   | 1.89                     | 0.54              |
| 1:AA:1152:A:OP1    | 10:AJ:70:HIS:ND1   | 2.40                     | 0.54              |
| 1:AA:1417:G:C6     | 1:AA:1482:G:C6     | 2.95                     | 0.54              |
| 1:AA:616:G:C2      | 1:AA:617:G:C8      | 2.95                     | 0.54              |
| 2:AB:27:MET:HG2    | 2:AB:189:THR:HA    | 1.89                     | 0.54              |
| 4:AD:123:ILE:N     | 4:AD:123:ILE:HD13  | 2.22                     | 0.54              |
| 4:AD:151:LYS:HB3   | 4:AD:178:MET:HE3   | 1.90                     | 0.54              |
| 10:AJ:73:LEU:O     | 10:AJ:74:VAL:HB    | 2.08                     | 0.54              |
| 13:AM:10:PRO:O     | 13:AM:11:ASP:HB3   | 2.07                     | 0.54              |
| 53:B5:50:ILE:HB    | 53:B5:52:PRO:HD3   | 1.89                     | 0.54              |
| 22:BA:1441:G:H2'   | 22:BA:1442:U:C6    | 2.42                     | 0.54              |
| 22:BA:2308:G:C5    | 27:BF:77:PHE:CE2   | 2.95                     | 0.54              |
| 22:BA:2511:U:O4    | 22:BA:2575:C:N3    | 2.40                     | 0.54              |
| 22:BA:627:A:C6     | 22:BA:637:A:C8     | 2.95                     | 0.54              |
| 29:BH:90:LEU:HA    | 29:BH:125:THR:HG23 | 1.89                     | 0.54              |
| 41:BT:17:SER:O     | 41:BT:18:GLU:C     | 2.45                     | 0.54              |
| 1:CA:1181:G:O2'    | 1:CA:1182:G:C8     | 2.56                     | 0.54              |
| 1:CA:66:A:H4'      | 1:CA:173:U:C5      | 2.42                     | 0.54              |
| 1:CA:736:C:H2'     | 1:CA:737:C:C6      | 2.42                     | 0.54              |
| 21:CU:12:PHE:O     | 21:CU:13:ASP:CB    | 2.54                     | 0.54              |
| 22:DA:1011:G:O2'   | 22:DA:1013:C:H5''  | 2.07                     | 0.54              |
| 22:DA:1316:U:C2    | 22:DA:1337:G:N2    | 2.76                     | 0.54              |
| 22:DA:1343:G:C6    | 22:DA:1344:U:O4    | 2.60                     | 0.54              |
| 22:DA:1428:C:O2'   | 22:DA:1569:A:OP2   | 2.20                     | 0.54              |
| 22:DA:1847:A:C2'   | 22:DA:1848:A:OP2   | 2.55                     | 0.54              |
| 22:DA:2267:A:H5''  | 22:DA:2268:A:C5'   | 2.38                     | 0.54              |
| 22:DA:792:A:H1'    | 22:DA:2072:C:O2'   | 2.07                     | 0.54              |
| 22:DA:867:C:C5     | 22:DA:868:U:C5     | 2.96                     | 0.54              |
| 24:DC:121:ASP:N    | 24:DC:121:ASP:OD1  | 2.41                     | 0.54              |
| 42:DU:34:VAL:HG22  | 42:DU:67:VAL:HG23  | 1.88                     | 0.54              |
| 1:AA:100:G:N7      | 1:AA:101:A:N7      | 2.55                     | 0.54              |
| 1:AA:769:G:H4'     | 1:AA:1513:A:H4'    | 1.89                     | 0.54              |
| 1:AA:258:G:C4      | 1:AA:259:G:C8      | 2.95                     | 0.54              |
| 1:AA:876:C:OP1     | 8:AH:76:GLN:NE2    | 2.40                     | 0.54              |
| 14:AN:20:TYR:O     | 14:AN:24:ARG:N     | 2.40                     | 0.54              |
| 15:AO:19:ALA:O     | 15:AO:20:ASN:CB    | 2.54                     | 0.54              |
| 19:AS:5:LEU:O      | 19:AS:7:LYS:N      | 2.40                     | 0.54              |
| 22:BA:1071:G:C8    | 22:BA:1089:A:N6    | 2.76                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:BA:1319:C:C2'  | 22:BA:1320:C:H5'  | 2.37                     | 0.54              |
| 22:BA:1583:A:O2'  | 22:BA:1584:U:O5'  | 2.25                     | 0.54              |
| 22:BA:1242:U:O2   | 33:BL:4:ASN:ND2   | 2.40                     | 0.54              |
| 34:BM:20:LEU:HD12 | 43:BV:81:PRO:HG2  | 1.88                     | 0.54              |
| 39:BR:14:VAL:HG11 | 39:BR:98:ILE:HG13 | 1.89                     | 0.54              |
| 44:BW:47:ALA:HB1  | 44:BW:51:VAL:O    | 2.07                     | 0.54              |
| 1:CA:1027:C:N4    | 1:CA:1034:G:N1    | 2.56                     | 0.54              |
| 1:CA:1296:C:C5'   | 1:CA:1297:G:OP2   | 2.55                     | 0.54              |
| 1:CA:203:G:N2     | 1:CA:215:C:N3     | 2.56                     | 0.54              |
| 1:CA:748:G:H2'    | 1:CA:749:A:H8     | 1.71                     | 0.54              |
| 2:CB:167:ASP:O    | 2:CB:168:HIS:HB3  | 2.07                     | 0.54              |
| 3:CC:42:TYR:CE1   | 3:CC:90:VAL:HG21  | 2.42                     | 0.54              |
| 4:CD:35:GLU:HG3   | 4:CD:36:GLN:N     | 2.22                     | 0.54              |
| 17:CQ:69:LYS:HG2  | 17:CQ:69:LYS:O    | 2.07                     | 0.54              |
| 21:CU:12:PHE:N    | 21:CU:12:PHE:CD1  | 2.74                     | 0.54              |
| 22:DA:104:A:H2'   | 22:DA:105:C:O4'   | 2.07                     | 0.54              |
| 22:DA:118:A:O4'   | 22:DA:178:G:O2'   | 2.24                     | 0.54              |
| 22:DA:1581:G:C5   | 22:DA:1582:C:N4   | 2.76                     | 0.54              |
| 22:DA:1856:U:O4   | 22:DA:1857:G:N1   | 2.41                     | 0.54              |
| 22:DA:2365:G:H4'  | 44:DW:60:PHE:CE2  | 2.42                     | 0.54              |
| 22:DA:2412:A:H3'  | 22:DA:2413:G:C8   | 2.43                     | 0.54              |
| 22:DA:303:G:C6    | 22:DA:304:U:N3    | 2.76                     | 0.54              |
| 24:DC:246:THR:C   | 24:DC:248:TRP:H   | 2.10                     | 0.54              |
| 22:DA:2019:A:H4'  | 38:DQ:34:VAL:HG21 | 1.90                     | 0.54              |
| 45:DX:33:LEU:HD23 | 45:DX:50:ARG:CZ   | 2.38                     | 0.54              |
| 1:AA:971:G:C8     | 1:AA:1365:G:H4'   | 2.43                     | 0.54              |
| 1:AA:173:U:C2     | 1:AA:197:A:N1     | 2.76                     | 0.54              |
| 1:AA:701:U:H4'    | 1:AA:702:A:H5''   | 1.89                     | 0.54              |
| 4:AD:174:ASP:O    | 4:AD:175:ALA:HB3  | 2.07                     | 0.54              |
| 22:BA:1098:A:C8   | 22:BA:1099:G:N7   | 2.76                     | 0.54              |
| 22:BA:2831:G:P    | 25:BD:56:LYS:NZ   | 2.80                     | 0.54              |
| 22:BA:538:A:H5''  | 31:BJ:7:LYS:HE3   | 1.89                     | 0.54              |
| 23:BB:54:G:H21    | 27:BF:26:MET:HE2  | 1.72                     | 0.54              |
| 29:BH:14:SER:OG   | 29:BH:17:ASP:CG   | 2.46                     | 0.54              |
| 1:CA:1235:U:H2'   | 1:CA:1236:A:O4'   | 2.07                     | 0.54              |
| 1:CA:369:G:OP2    | 1:CA:388:G:N1     | 2.39                     | 0.54              |
| 1:CA:374:A:H5''   | 1:CA:452:A:C2     | 2.43                     | 0.54              |
| 1:CA:632:U:O2     | 1:CA:632:U:C2'    | 2.56                     | 0.54              |
| 1:CA:743:A:C6     | 1:CA:744:C:C4     | 2.96                     | 0.54              |
| 1:CA:1202:U:N3    | 14:CN:82:ILE:HG21 | 2.22                     | 0.54              |
| 14:CN:87:ALA:O    | 14:CN:90:ARG:N    | 2.41                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 19:CS:73:GLU:HB2   | 19:CS:74:PHE:CD1   | 2.42                     | 0.54              |
| 20:CT:60:ARG:O     | 20:CT:64:LYS:N     | 2.38                     | 0.54              |
| 51:D3:31:HIS:ND1   | 51:D3:32:ILE:HG13  | 2.22                     | 0.54              |
| 22:DA:1027:A:C6    | 22:DA:1126:A:C4    | 2.95                     | 0.54              |
| 22:DA:1343:G:N2    | 22:DA:1405:U:C2    | 2.76                     | 0.54              |
| 22:DA:1693:U:OP2   | 22:DA:1694:C:N4    | 2.37                     | 0.54              |
| 22:DA:2326:C:H1'   | 22:DA:2327:A:OP1   | 2.08                     | 0.54              |
| 22:DA:2849:U:H4'   | 22:DA:2868:A:C2    | 2.43                     | 0.54              |
| 22:DA:471:A:OP1    | 26:DE:79:ARG:NH1   | 2.41                     | 0.54              |
| 22:DA:479:A:H4'    | 22:DA:480:A:OP1    | 2.08                     | 0.54              |
| 27:DF:5:HIS:O      | 27:DF:9:LYS:HG3    | 2.07                     | 0.54              |
| 33:DL:100:ILE:HG13 | 33:DL:100:ILE:O    | 2.07                     | 0.54              |
| 38:DQ:72:ASN:HB3   | 38:DQ:110:VAL:HG11 | 1.89                     | 0.54              |
| 1:AA:1118:U:H1'    | 1:AA:1179:A:C4     | 2.42                     | 0.54              |
| 3:AC:79:LYS:O      | 3:AC:82:GLU:HG3    | 2.06                     | 0.54              |
| 7:AG:15:ASP:OD2    | 7:AG:44:TYR:OH     | 2.26                     | 0.54              |
| 7:AG:49:THR:O      | 7:AG:53:ARG:CB     | 2.56                     | 0.54              |
| 7:AG:74:GLU:HG2    | 7:AG:91:VAL:HB     | 1.90                     | 0.54              |
| 10:AJ:28:THR:O     | 10:AJ:28:THR:HG22  | 2.07                     | 0.54              |
| 10:AJ:6:ILE:HD12   | 10:AJ:76:ILE:HB    | 1.90                     | 0.54              |
| 16:AP:51:ARG:HH11  | 16:AP:51:ARG:HG2   | 1.71                     | 0.54              |
| 51:B3:31:HIS:CD2   | 51:B3:31:HIS:C     | 2.80                     | 0.54              |
| 22:BA:1355:G:C2'   | 22:BA:1356:G:H5'   | 2.38                     | 0.54              |
| 22:BA:2328:A:H2'   | 22:BA:2329:U:C6    | 2.43                     | 0.54              |
| 22:BA:2869:G:H2'   | 22:BA:2870:C:O4'   | 2.08                     | 0.54              |
| 22:BA:360:U:H3'    | 22:BA:361:G:C8     | 2.42                     | 0.54              |
| 22:BA:813:U:H2'    | 22:BA:814:C:H6     | 1.72                     | 0.54              |
| 22:BA:998:C:H2'    | 22:BA:999:U:O5'    | 2.07                     | 0.54              |
| 22:BA:1993:U:H4'   | 25:BD:133:THR:HG21 | 1.90                     | 0.54              |
| 29:BH:103:VAL:HG21 | 29:BH:132:PHE:CE1  | 2.42                     | 0.54              |
| 29:BH:77:THR:O     | 29:BH:77:THR:CG2   | 2.56                     | 0.54              |
| 30:BI:116:ASP:O    | 30:BI:117:MET:CB   | 2.56                     | 0.54              |
| 46:BY:18:LEU:O     | 46:BY:22:LEU:N     | 2.38                     | 0.54              |
| 1:CA:1386:G:C2     | 1:CA:1387:G:C8     | 2.96                     | 0.54              |
| 1:CA:1513:A:H2'    | 1:CA:1514:G:C8     | 2.43                     | 0.54              |
| 1:CA:237:G:C6      | 1:CA:238:A:C5      | 2.95                     | 0.54              |
| 1:CA:818:G:O2'     | 1:CA:819:A:H5'     | 2.07                     | 0.54              |
| 4:CD:147:GLU:O     | 4:CD:150:LYS:HB3   | 2.07                     | 0.54              |
| 9:CI:118:LEU:HD23  | 9:CI:121:ALA:O     | 2.08                     | 0.54              |
| 22:DA:1054:A:H2'   | 22:DA:1055:G:C8    | 2.43                     | 0.54              |
| 22:DA:125:A:OP2    | 50:D2:19:ARG:NH2   | 2.41                     | 0.54              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:DA:1364:G:C6    | 22:DA:1368:G:C6    | 2.95                     | 0.54              |
| 22:DA:192:C:P      | 57:DA:3739:HOH:O   | 2.65                     | 0.54              |
| 22:DA:2038:G:H2'   | 22:DA:2039:U:O4'   | 2.07                     | 0.54              |
| 22:DA:2297:A:H2'   | 22:DA:2297:A:N3    | 2.23                     | 0.54              |
| 22:DA:2308:G:H5'   | 22:DA:2309:A:OP2   | 2.08                     | 0.54              |
| 22:DA:2448:A:HO2'  | 22:DA:2449:U:H5    | 1.50                     | 0.54              |
| 22:DA:425:G:N2     | 22:DA:426:C:N3     | 2.56                     | 0.54              |
| 22:DA:528:A:H2'    | 22:DA:529:A:H5''   | 1.89                     | 0.54              |
| 41:DT:61:LEU:HD12  | 41:DT:62:VAL:N     | 2.23                     | 0.54              |
| 1:AA:1452:C:O4'    | 1:AA:1453:G:C2     | 2.61                     | 0.54              |
| 1:AA:259:G:N2      | 1:AA:260:G:H1'     | 2.22                     | 0.54              |
| 10:AJ:51:VAL:HB    | 14:AN:81:ARG:HB2   | 1.90                     | 0.54              |
| 22:BA:1737:G:C6    | 22:BA:1738:G:N1    | 2.75                     | 0.54              |
| 27:BF:25:VAL:O     | 27:BF:28:VAL:HG12  | 2.07                     | 0.54              |
| 1:CA:252:U:O4      | 1:CA:253:A:N6      | 2.40                     | 0.54              |
| 6:CF:81:ASN:OD1    | 6:CF:81:ASN:C      | 2.45                     | 0.54              |
| 11:CK:107:ILE:O    | 11:CK:107:ILE:HG23 | 2.06                     | 0.54              |
| 19:CS:22:ALA:CB    | 19:CS:47:LEU:HD13  | 2.37                     | 0.54              |
| 22:DA:1529:G:O6    | 22:DA:1543:G:C2    | 2.60                     | 0.54              |
| 22:DA:2563:U:H1'   | 22:DA:2566:A:N6    | 2.23                     | 0.54              |
| 22:DA:2615:U:C2    | 48:D0:4:GLN:HA     | 2.43                     | 0.54              |
| 22:DA:2688:G:N1    | 22:DA:2720:U:OP2   | 2.31                     | 0.54              |
| 22:DA:370:G:O2'    | 22:DA:423:A:H3'    | 2.06                     | 0.54              |
| 35:DN:12:ARG:HG2   | 35:DN:16:HIS:HB3   | 1.89                     | 0.54              |
| 1:AA:1435:G:H2'    | 1:AA:1436:U:C6     | 2.42                     | 0.54              |
| 10:AJ:66:GLU:HB3   | 14:AN:99:ALA:CB    | 2.38                     | 0.54              |
| 53:B5:100:ILE:HG22 | 53:B5:104:ILE:CB   | 2.38                     | 0.54              |
| 22:BA:2014:A:H2'   | 22:BA:2015:A:C8    | 2.43                     | 0.54              |
| 22:BA:63:A:C2      | 22:BA:64:A:C5      | 2.96                     | 0.54              |
| 32:BK:36:GLY:HA2   | 32:BK:62:VAL:O     | 2.08                     | 0.54              |
| 1:CA:1000:A:H2'    | 1:CA:1001:C:O4'    | 2.08                     | 0.54              |
| 1:CA:528:C:O2      | 1:CA:528:C:H2'     | 2.08                     | 0.54              |
| 1:CA:749:A:O2'     | 1:CA:750:C:H5'     | 2.08                     | 0.54              |
| 1:CA:779:C:H2'     | 1:CA:780:A:H5'     | 1.88                     | 0.54              |
| 1:CA:853:C:C4      | 1:CA:854:U:C5      | 2.95                     | 0.54              |
| 1:CA:890:G:N2      | 1:CA:906:A:H2'     | 2.23                     | 0.54              |
| 2:CB:85:LEU:HG     | 2:CB:85:LEU:O      | 2.08                     | 0.54              |
| 3:CC:43:LEU:HD21   | 3:CC:68:ILE:HD11   | 1.88                     | 0.54              |
| 4:CD:196:ASN:HB3   | 4:CD:198:HIS:CE1   | 2.42                     | 0.54              |
| 5:CE:150:PRO:C     | 5:CE:152:MET:H     | 2.10                     | 0.54              |
| 11:CK:18:ASP:HB3   | 11:CK:81:ASN:OD1   | 2.07                     | 0.54              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 17:CQ:70:THR:O      | 17:CQ:71:LYS:C     | 2.46                     | 0.54              |
| 20:CT:55:GLN:N      | 20:CT:56:PRO:HD2   | 2.23                     | 0.54              |
| 21:CU:36:GLU:HG3    | 21:CU:37:PHE:H     | 1.72                     | 0.54              |
| 22:DA:1230:A:H2'    | 22:DA:1231:U:C6    | 2.43                     | 0.54              |
| 22:DA:1245:G:H4'    | 26:DE:33:VAL:HG11  | 1.88                     | 0.54              |
| 22:DA:1345:C:H5'    | 22:DA:1396:U:O4    | 2.06                     | 0.54              |
| 22:DA:19:A:C2       | 22:DA:522:A:C2     | 2.96                     | 0.54              |
| 22:DA:1782:U:O4     | 22:DA:2586:U:H5    | 1.89                     | 0.54              |
| 22:DA:2814:A:C6     | 22:DA:2815:C:C4    | 2.95                     | 0.54              |
| 55:DA:3001:DOL:H432 | 55:DA:3001:DOL:N5  | 2.22                     | 0.54              |
| 24:DC:108:LYS:HA    | 24:DC:196:GLY:HA3  | 1.89                     | 0.54              |
| 24:DC:267:ILE:O     | 24:DC:267:ILE:HG22 | 2.06                     | 0.54              |
| 24:DC:43:ARG:NH2    | 24:DC:49:ILE:HD11  | 2.23                     | 0.54              |
| 39:DR:80:ARG:C      | 39:DR:82:HIS:H     | 2.11                     | 0.54              |
| 1:AA:66:A:O4'       | 1:AA:173:U:C4      | 2.61                     | 0.54              |
| 1:AA:705:G:C5       | 1:AA:706:A:C8      | 2.96                     | 0.54              |
| 1:AA:723:U:H2'      | 1:AA:855:U:H4'     | 1.90                     | 0.54              |
| 13:AM:73:ILE:O      | 13:AM:76:SER:OG    | 2.25                     | 0.54              |
| 22:BA:1794:A:H2'    | 22:BA:1795:C:C6    | 2.42                     | 0.54              |
| 22:BA:283:G:N7      | 22:BA:284:U:C5     | 2.76                     | 0.54              |
| 22:BA:560:C:O2      | 38:BQ:48:ARG:NH1   | 2.39                     | 0.54              |
| 23:BB:42:C:C6       | 27:BF:66:LEU:HD13  | 2.42                     | 0.54              |
| 26:BE:119:ILE:HB    | 26:BE:187:VAL:HG22 | 1.88                     | 0.54              |
| 27:BF:173:PHE:O     | 27:BF:175:PHE:N    | 2.40                     | 0.54              |
| 30:BI:21:SER:N      | 30:BI:22:PRO:CD    | 2.71                     | 0.54              |
| 1:CA:142:G:C2       | 1:CA:143:A:H1'     | 2.42                     | 0.54              |
| 1:CA:780:A:C2       | 1:CA:803:G:N1      | 2.76                     | 0.54              |
| 10:CJ:92:LEU:O      | 10:CJ:93:ALA:HB2   | 2.08                     | 0.54              |
| 22:DA:1476:U:H1'    | 22:DA:1732:C:C2    | 2.43                     | 0.54              |
| 22:DA:2214:C:H2'    | 22:DA:2215:C:O5'   | 2.08                     | 0.54              |
| 22:DA:2552:U:C2     | 22:DA:2554:U:C5'   | 2.91                     | 0.54              |
| 22:DA:289:G:N2      | 22:DA:352:A:C2     | 2.76                     | 0.54              |
| 22:DA:586:A:H1'     | 22:DA:672:C:H1'    | 1.89                     | 0.54              |
| 25:DD:187:LEU:CD2   | 25:DD:203:VAL:HG11 | 2.38                     | 0.54              |
| 26:DE:77:ILE:HG13   | 26:DE:77:ILE:O     | 2.08                     | 0.54              |
| 22:DA:588:U:H1'     | 26:DE:85:PHE:CD1   | 2.43                     | 0.54              |
| 47:DZ:13:ALA:HB2    | 47:DZ:24:LEU:CD1   | 2.38                     | 0.54              |
| 4:AD:29:ASP:C       | 4:AD:30:THR:O      | 2.43                     | 0.54              |
| 5:AE:108:GLY:O      | 5:AE:109:GLY:C     | 2.47                     | 0.54              |
| 5:AE:119:GLY:O      | 5:AE:121:HIS:ND1   | 2.41                     | 0.54              |
| 1:AA:826:C:H5'      | 8:AH:13:ARG:NH1    | 2.22                     | 0.54              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:AI:58:VAL:O     | 9:AI:59:GLU:HG2   | 2.08                     | 0.54              |
| 12:AL:76:GLU:O    | 12:AL:77:HIS:HB2  | 2.07                     | 0.54              |
| 20:AT:83:ILE:HD12 | 20:AT:84:ASN:N    | 2.22                     | 0.54              |
| 22:BA:1413:A:H2'  | 22:BA:1414:C:O4'  | 2.08                     | 0.54              |
| 22:BA:1474:U:C3'  | 22:BA:1475:G:H5'  | 2.38                     | 0.54              |
| 22:BA:1607:C:N4   | 22:BA:1622:G:N7   | 2.57                     | 0.54              |
| 22:BA:1782:U:OP1  | 57:BA:3693:HOH:O  | 2.19                     | 0.54              |
| 22:BA:2532:G:N2   | 22:BA:2663:G:O2'  | 2.41                     | 0.54              |
| 22:BA:388:G:N7    | 22:BA:390:U:H2'   | 2.22                     | 0.54              |
| 36:BO:100:HIS:O   | 36:BO:104:GLN:HB3 | 2.08                     | 0.54              |
| 1:CA:1041:G:C6    | 1:CA:1042:A:N6    | 2.75                     | 0.54              |
| 4:CD:168:PRO:HB2  | 4:CD:171:LEU:HD12 | 1.90                     | 0.54              |
| 5:CE:137:VAL:O    | 5:CE:138:ARG:CB   | 2.56                     | 0.54              |
| 16:CP:19:VAL:HG13 | 16:CP:37:GLY:N    | 2.22                     | 0.54              |
| 17:CQ:8:LEU:HD13  | 17:CQ:73:TRP:CZ3  | 2.43                     | 0.54              |
| 18:CR:22:ASP:OD2  | 18:CR:24:LYS:NZ   | 2.41                     | 0.54              |
| 22:DA:1182:G:H2'  | 22:DA:1183:U:O4'  | 2.08                     | 0.54              |
| 22:DA:1445:G:C2   | 22:DA:1547:C:N3   | 2.76                     | 0.54              |
| 22:DA:2480:C:N4   | 22:DA:2481:G:C6   | 2.76                     | 0.54              |
| 22:DA:607:U:H5    | 22:DA:619:G:C5    | 2.26                     | 0.54              |
| 22:DA:694:U:C3'   | 22:DA:695:G:H5''  | 2.38                     | 0.54              |
| 22:DA:71:A:H5'    | 22:DA:73:A:C4     | 2.43                     | 0.54              |
| 23:DB:80:U:H2'    | 23:DB:81:G:C8     | 2.43                     | 0.54              |
| 22:DA:1566:A:C2   | 24:DC:213:TRP:CE3 | 2.95                     | 0.54              |
| 22:DA:2751:G:OP1  | 28:DG:3:ARG:NH1   | 2.41                     | 0.54              |
| 35:DN:69:ARG:O    | 35:DN:70:THR:HG23 | 2.08                     | 0.54              |
| 1:AA:1182:G:H4'   | 1:AA:1183:U:H5'   | 1.90                     | 0.53              |
| 1:AA:260:G:H2'    | 1:AA:261:U:C6     | 2.42                     | 0.53              |
| 1:AA:858:G:C2'    | 1:AA:859:G:H5'    | 2.38                     | 0.53              |
| 1:AA:874:G:C6     | 1:AA:875:U:C4     | 2.96                     | 0.53              |
| 1:AA:90:C:C2      | 1:AA:91:U:C5      | 2.96                     | 0.53              |
| 2:AB:51:ASN:O     | 2:AB:52:GLU:HB2   | 2.09                     | 0.53              |
| 5:AE:155:ALA:HB1  | 8:AH:66:PHE:CZ    | 2.43                     | 0.53              |
| 12:AL:39:THR:OG1  | 12:AL:39:THR:O    | 2.20                     | 0.53              |
| 22:BA:1315:C:C2   | 22:BA:1338:G:N2   | 2.76                     | 0.53              |
| 22:BA:528:A:H2'   | 22:BA:529:A:H5''  | 1.90                     | 0.53              |
| 22:BA:974:G:H8    | 22:BA:990:A:N6    | 2.01                     | 0.53              |
| 22:BA:1997:C:OP2  | 25:BD:129:THR:CG2 | 2.57                     | 0.53              |
| 37:BP:22:PRO:HD3  | 37:BP:50:ILE:HD12 | 1.90                     | 0.53              |
| 38:BQ:105:ALA:O   | 38:BQ:108:ALA:HB3 | 2.07                     | 0.53              |
| 46:BY:9:LYS:HB3   | 46:BY:12:GLU:CG   | 2.38                     | 0.53              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:CA:425:G:H2'     | 1:CA:426:U:O4'    | 2.08                     | 0.53              |
| 7:CG:92:ARG:NE     | 7:CG:93:PRO:CD    | 2.71                     | 0.53              |
| 9:CI:21:ILE:HG12   | 9:CI:62:ASP:O     | 2.07                     | 0.53              |
| 1:CA:562:U:H2'     | 12:CL:14:ARG:HD3  | 1.89                     | 0.53              |
| 22:DA:2742:G:H5''  | 52:D4:1:MET:HE1   | 1.89                     | 0.53              |
| 22:DA:1715:G:O2'   | 22:DA:1716:U:OP2  | 2.25                     | 0.53              |
| 22:DA:2058:A:C6    | 22:DA:2059:A:N6   | 2.76                     | 0.53              |
| 22:DA:359:G:H2'    | 22:DA:360:U:O4'   | 2.08                     | 0.53              |
| 22:DA:630:G:C3'    | 22:DA:631:A:H5''  | 2.38                     | 0.53              |
| 22:DA:813:U:H2'    | 22:DA:814:C:C6    | 2.42                     | 0.53              |
| 25:DD:133:THR:HG23 | 25:DD:134:HIS:N   | 2.24                     | 0.53              |
| 1:AA:1157:A:C5     | 1:AA:1180:A:C6    | 2.95                     | 0.53              |
| 1:AA:211:G:N2      | 1:AA:212:G:C8     | 2.76                     | 0.53              |
| 1:AA:58:C:O2'      | 1:AA:59:A:H5'     | 2.06                     | 0.53              |
| 1:AA:266:G:H3'     | 17:AQ:69:LYS:HB3  | 1.91                     | 0.53              |
| 22:BA:589:U:H2'    | 22:BA:590:A:C8    | 2.43                     | 0.53              |
| 34:BM:12:MET:CE    | 34:BM:71:LYS:HG3  | 2.38                     | 0.53              |
| 38:BQ:36:PHE:CZ    | 38:BQ:40:ILE:HD11 | 2.43                     | 0.53              |
| 1:CA:121:U:H3'     | 1:CA:122:G:H5'    | 1.91                     | 0.53              |
| 1:CA:805:C:C2      | 1:CA:806:C:C5     | 2.96                     | 0.53              |
| 6:CF:8:PHE:CE2     | 6:CF:60:VAL:HB    | 2.42                     | 0.53              |
| 6:CF:98:GLU:O      | 6:CF:99:ALA:CB    | 2.56                     | 0.53              |
| 12:CL:25:GLU:C     | 12:CL:27:CYS:N    | 2.59                     | 0.53              |
| 19:CS:6:LYS:CB     | 19:CS:7:LYS:HE2   | 2.37                     | 0.53              |
| 22:DA:1378:A:C2'   | 22:DA:1380:G:N7   | 2.71                     | 0.53              |
| 22:DA:2146:C:H4'   | 22:DA:2147:A:OP1  | 2.07                     | 0.53              |
| 22:DA:2214:C:C2'   | 22:DA:2215:C:O5'  | 2.56                     | 0.53              |
| 22:DA:2747:G:O2'   | 28:DG:67:THR:HG22 | 2.08                     | 0.53              |
| 22:DA:291:G:N2     | 22:DA:350:G:C5    | 2.77                     | 0.53              |
| 23:DB:62:C:H2'     | 23:DB:63:C:C6     | 2.42                     | 0.53              |
| 24:DC:251:GLN:NE2  | 24:DC:253:LYS:O   | 2.41                     | 0.53              |
| 41:DT:10:VAL:HG12  | 41:DT:11:LEU:N    | 2.23                     | 0.53              |
| 1:AA:1160:G:O2'    | 1:AA:1161:C:P     | 2.67                     | 0.53              |
| 1:AA:195:A:H1'     | 1:AA:222:C:O2'    | 2.08                     | 0.53              |
| 3:AC:7:PRO:HG2     | 3:AC:184:TYR:CG   | 2.43                     | 0.53              |
| 13:AM:3:ARG:O      | 13:AM:4:ILE:HG12  | 2.08                     | 0.53              |
| 20:AT:44:LYS:CB    | 20:AT:87:ALA:HB1  | 2.39                     | 0.53              |
| 11:AK:126:LYS:CA   | 21:AU:34:ARG:HH21 | 2.21                     | 0.53              |
| 49:B1:52:ALA:O     | 49:B1:53:LYS:OXT  | 2.27                     | 0.53              |
| 22:BA:1417:C:H2'   | 22:BA:1418:G:O4'  | 2.08                     | 0.53              |
| 22:BA:1916:A:C6    | 22:BA:1917:U:C2   | 2.96                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:BA:198:C:P      | 57:BA:3760:HOH:O   | 2.64                     | 0.53              |
| 22:BA:228:C:H4'    | 22:BA:229:C:H5''   | 1.90                     | 0.53              |
| 22:BA:2329:U:H2'   | 22:BA:2330:G:C8    | 2.43                     | 0.53              |
| 22:BA:2748:A:H1'   | 28:BG:67:THR:HG22  | 1.90                     | 0.53              |
| 22:BA:2683:C:H4'   | 25:BD:13:ARG:NH1   | 2.23                     | 0.53              |
| 26:BE:149:ILE:C    | 26:BE:149:ILE:HD12 | 2.29                     | 0.53              |
| 22:BA:585:G:N7     | 38:BQ:6:ARG:NH1    | 2.56                     | 0.53              |
| 1:CA:1201:A:H4'    | 1:CA:1202:U:O5'    | 2.08                     | 0.53              |
| 1:CA:242:G:N2      | 1:CA:285:C:C2      | 2.77                     | 0.53              |
| 3:CC:162:ILE:HD12  | 3:CC:162:ILE:O     | 2.08                     | 0.53              |
| 7:CG:78:ARG:O      | 7:CG:79:ARG:HB2    | 2.08                     | 0.53              |
| 22:DA:1435:G:C2'   | 22:DA:1436:G:H5'   | 2.38                     | 0.53              |
| 22:DA:1441:G:H2'   | 22:DA:1442:U:C6    | 2.43                     | 0.53              |
| 22:DA:1605:C:H2'   | 22:DA:1606:C:H5'   | 1.89                     | 0.53              |
| 22:DA:1814:G:C6    | 22:DA:1815:A:C6    | 2.96                     | 0.53              |
| 22:DA:185:G:N1     | 22:DA:212:G:C2     | 2.76                     | 0.53              |
| 22:DA:2815:C:O2'   | 48:D0:41:HIS:ND1   | 2.40                     | 0.53              |
| 22:DA:548:G:H4'    | 22:DA:549:G:C2     | 2.43                     | 0.53              |
| 22:DA:704:G:H1'    | 22:DA:726:G:H22    | 1.73                     | 0.53              |
| 22:DA:776:G:C8     | 22:DA:793:A:C4     | 2.95                     | 0.53              |
| 22:DA:852:U:H2'    | 22:DA:853:C:O4'    | 2.09                     | 0.53              |
| 25:DD:32:ASN:HB3   | 25:DD:50:VAL:HB    | 1.90                     | 0.53              |
| 22:DA:600:G:C5'    | 26:DE:27:LEU:HD22  | 2.37                     | 0.53              |
| 30:DI:62:TYR:HB2   | 30:DI:66:SER:O     | 2.08                     | 0.53              |
| 22:DA:1246:A:OP2   | 33:DL:13:LYS:NZ    | 2.41                     | 0.53              |
| 36:DO:49:VAL:HG21  | 36:DO:82:ALA:HA    | 1.91                     | 0.53              |
| 47:DZ:7:ILE:N      | 47:DZ:36:VAL:O     | 2.40                     | 0.53              |
| 1:AA:1064:G:O4'    | 1:AA:1066:C:C6     | 2.61                     | 0.53              |
| 1:AA:1352:C:H2'    | 1:AA:1353:G:C8     | 2.44                     | 0.53              |
| 1:AA:203:G:O2'     | 1:AA:465:A:N1      | 2.36                     | 0.53              |
| 1:AA:659:U:C2      | 1:AA:660:C:C6      | 2.96                     | 0.53              |
| 17:AQ:16:LYS:HG3   | 17:AQ:16:LYS:O     | 2.07                     | 0.53              |
| 22:BA:948:C:O2     | 22:BA:984:A:O2'    | 2.26                     | 0.53              |
| 23:BB:14:U:O2      | 23:BB:107:G:H4'    | 2.09                     | 0.53              |
| 26:BE:108:ILE:HD11 | 26:BE:180:LEU:HD13 | 1.90                     | 0.53              |
| 1:CA:572:A:H5'     | 1:CA:573:A:OP2     | 2.08                     | 0.53              |
| 1:CA:748:G:H2'     | 1:CA:749:A:C8      | 2.44                     | 0.53              |
| 4:CD:35:GLU:HG3    | 4:CD:36:GLN:HG3    | 1.90                     | 0.53              |
| 7:CG:5:ARG:HE      | 7:CG:5:ARG:HA      | 1.72                     | 0.53              |
| 51:D3:32:ILE:HG22  | 51:D3:32:ILE:O     | 2.07                     | 0.53              |
| 22:DA:747:U:O2     | 22:DA:2014:A:H1'   | 2.07                     | 0.53              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 22:DA:2209:G:C5    | 22:DA:2210:U:C4   | 2.97                     | 0.53              |
| 22:DA:30:G:H2'     | 22:DA:31:C:O4'    | 2.09                     | 0.53              |
| 22:DA:392:U:H2'    | 22:DA:393:C:C6    | 2.43                     | 0.53              |
| 22:DA:981:A:H5''   | 57:DA:3588:HOH:O  | 2.08                     | 0.53              |
| 22:DA:2882:A:H5'   | 35:DN:96:ARG:HB2  | 1.90                     | 0.53              |
| 38:DQ:10:ALA:O     | 38:DQ:13:ARG:HG3  | 2.08                     | 0.53              |
| 1:AA:1031:C:H4'    | 1:AA:1032:G:O5'   | 2.08                     | 0.53              |
| 1:AA:9:G:OP2       | 5:AE:126:LYS:HG3  | 2.09                     | 0.53              |
| 4:AD:138:SER:HB2   | 4:AD:139:PRO:HD2  | 1.89                     | 0.53              |
| 6:AF:16:GLU:HB3    | 4:CD:189:SER:HA   | 1.91                     | 0.53              |
| 6:AF:15:SER:O      | 6:AF:18:VAL:HG23  | 2.09                     | 0.53              |
| 6:AF:4:TYR:CD2     | 6:AF:71:ILE:HD13  | 2.44                     | 0.53              |
| 6:AF:92:THR:O      | 6:AF:93:LYS:HG2   | 2.07                     | 0.53              |
| 7:AG:13:LEU:HD22   | 7:AG:13:LEU:N     | 2.24                     | 0.53              |
| 9:AI:30:ILE:O      | 9:AI:33:ARG:HB2   | 2.08                     | 0.53              |
| 13:AM:27:LYS:O     | 13:AM:31:LYS:HG3  | 2.08                     | 0.53              |
| 22:BA:1288:G:C4    | 22:BA:1327:A:C2   | 2.96                     | 0.53              |
| 22:BA:1464:G:H2'   | 22:BA:1465:G:C8   | 2.43                     | 0.53              |
| 22:BA:1735:A:C2    | 22:BA:1736:U:H1'  | 2.43                     | 0.53              |
| 22:BA:630:G:N2     | 22:BA:633:A:OP2   | 2.40                     | 0.53              |
| 26:BE:149:ILE:HD12 | 26:BE:150:THR:N   | 2.23                     | 0.53              |
| 30:BI:69:PHE:CD1   | 30:BI:69:PHE:O    | 2.62                     | 0.53              |
| 35:BN:28:LEU:O     | 35:BN:32:GLU:N    | 2.42                     | 0.53              |
| 35:BN:2:ARG:HA     | 35:BN:5:LYS:HD2   | 1.91                     | 0.53              |
| 38:BQ:24:TYR:O     | 38:BQ:25:TYR:CB   | 2.57                     | 0.53              |
| 1:CA:1387:G:H2'    | 1:CA:1388:C:C6    | 2.43                     | 0.53              |
| 1:CA:1491:G:H3'    | 1:CA:1492:A:C8    | 2.44                     | 0.53              |
| 1:CA:374:A:C2      | 1:CA:375:U:C6     | 2.96                     | 0.53              |
| 5:CE:38:VAL:HG12   | 5:CE:117:VAL:HG21 | 1.91                     | 0.53              |
| 9:CI:88:MET:O      | 9:CI:88:MET:HG2   | 2.08                     | 0.53              |
| 11:CK:45:ALA:HB3   | 11:CK:70:CYS:HB2  | 1.90                     | 0.53              |
| 13:CM:114:LYS:HB2  | 13:CM:115:PRO:HD3 | 1.90                     | 0.53              |
| 22:DA:1077:A:C2    | 22:DA:1088:A:C2   | 2.97                     | 0.53              |
| 22:DA:1154:G:OP1   | 38:DQ:58:ARG:HD3  | 2.08                     | 0.53              |
| 22:DA:1343:G:C5    | 22:DA:1344:U:C4   | 2.96                     | 0.53              |
| 22:DA:1645:G:H5''  | 22:DA:1646:C:O5'  | 2.09                     | 0.53              |
| 22:DA:2103:C:H2'   | 22:DA:2104:C:C6   | 2.43                     | 0.53              |
| 22:DA:2831:G:OP1   | 25:DD:56:LYS:NZ   | 2.36                     | 0.53              |
| 22:DA:693:A:C5     | 22:DA:694:U:C4    | 2.97                     | 0.53              |
| 22:DA:720:U:H2'    | 22:DA:721:A:C8    | 2.43                     | 0.53              |
| 24:DC:147:LYS:HB2  | 24:DC:150:LYS:HB2 | 1.91                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 26:DE:8:ALA:HB2   | 26:DE:122:GLU:HG3 | 1.91                     | 0.53              |
| 1:AA:390:U:H2'    | 1:AA:391:G:C8     | 2.44                     | 0.53              |
| 1:AA:771:G:O2'    | 1:AA:772:U:H5'    | 2.08                     | 0.53              |
| 1:AA:872:A:C4     | 1:AA:874:G:N7     | 2.77                     | 0.53              |
| 12:AL:44:LYS:HB2  | 12:AL:45:PRO:CD   | 2.38                     | 0.53              |
| 18:AR:26:ILE:O    | 18:AR:30:LYS:HG3  | 2.08                     | 0.53              |
| 1:AA:322:C:O2'    | 20:AT:18:ARG:HG3  | 2.08                     | 0.53              |
| 20:AT:67:ILE:HG13 | 20:AT:71:LYS:HG2  | 1.89                     | 0.53              |
| 22:BA:1224:U:C4   | 22:BA:1225:G:C6   | 2.96                     | 0.53              |
| 22:BA:1584:U:O2   | 22:BA:1584:U:C2'  | 2.56                     | 0.53              |
| 22:BA:1936:A:C2   | 22:BA:1945:G:C8   | 2.97                     | 0.53              |
| 22:BA:2070:A:C2   | 22:BA:2442:C:C2   | 2.97                     | 0.53              |
| 38:BQ:50:ARG:O    | 38:BQ:54:LYS:HE3  | 2.08                     | 0.53              |
| 39:BR:21:ARG:CZ   | 39:BR:93:PHE:CE1  | 2.91                     | 0.53              |
| 1:CA:256:U:H2'    | 1:CA:257:G:O4'    | 2.08                     | 0.53              |
| 1:CA:355:C:C4     | 1:CA:356:A:N7     | 2.77                     | 0.53              |
| 1:CA:632:U:H3'    | 1:CA:633:G:H5'    | 1.90                     | 0.53              |
| 1:CA:664:G:H2'    | 1:CA:666:G:OP1    | 2.08                     | 0.53              |
| 1:CA:892:A:C5     | 1:CA:893:C:C5     | 2.96                     | 0.53              |
| 2:CB:102:THR:HB   | 2:CB:175:GLU:HG3  | 1.91                     | 0.53              |
| 1:CA:1126:U:O4    | 10:CJ:73:LEU:HD12 | 2.09                     | 0.53              |
| 10:CJ:83:THR:O    | 10:CJ:87:LEU:HD12 | 2.08                     | 0.53              |
| 49:D1:50:LYS:O    | 49:D1:51:GLU:HB3  | 2.07                     | 0.53              |
| 51:D3:31:HIS:CE1  | 51:D3:32:ILE:CD1  | 2.92                     | 0.53              |
| 22:DA:1223:G:N2   | 22:DA:1225:G:H3'  | 2.23                     | 0.53              |
| 22:DA:1301:A:H2'  | 22:DA:1301:A:N3   | 2.24                     | 0.53              |
| 22:DA:1330:C:C2'  | 22:DA:1331:G:O5'  | 2.57                     | 0.53              |
| 22:DA:1362:C:C2'  | 22:DA:1363:C:H5'  | 2.38                     | 0.53              |
| 22:DA:1566:A:C2   | 24:DC:213:TRP:CG  | 2.97                     | 0.53              |
| 22:DA:2720:U:C6   | 22:DA:2872:A:N1   | 2.77                     | 0.53              |
| 29:DH:2:GLN:O     | 29:DH:3:VAL:HG22  | 2.09                     | 0.53              |
| 29:DH:32:PRO:O    | 29:DH:33:GLN:HB2  | 2.09                     | 0.53              |
| 31:DJ:58:ASN:OD1  | 31:DJ:127:GLY:O   | 2.26                     | 0.53              |
| 22:DA:626:A:C2    | 33:DL:78:ARG:HD3  | 2.43                     | 0.53              |
| 35:DN:20:MET:HG3  | 35:DN:21:PHE:CD1  | 2.43                     | 0.53              |
| 35:DN:28:LEU:HG   | 35:DN:28:LEU:O    | 2.07                     | 0.53              |
| 22:DA:2840:C:H5'' | 35:DN:53:THR:OG1  | 2.08                     | 0.53              |
| 44:DW:50:ASN:OD1  | 44:DW:63:ALA:HB2  | 2.09                     | 0.53              |
| 1:AA:1179:A:H2'   | 1:AA:1180:A:O4'   | 2.07                     | 0.53              |
| 1:AA:1296:C:H4'   | 1:AA:1302:C:C4    | 2.43                     | 0.53              |
| 1:AA:1446:A:C2'   | 1:AA:1447:A:H5'   | 2.39                     | 0.53              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 5:AE:41:ASP:OD1   | 5:AE:42:GLY:N      | 2.42                     | 0.53              |
| 13:AM:83:LEU:HD21 | 19:AS:65:GLU:HG2   | 1.89                     | 0.53              |
| 20:AT:58:VAL:CG1  | 20:AT:72:ALA:HB1   | 2.38                     | 0.53              |
| 53:B5:204:GLY:O   | 53:B5:205:ALA:HB3  | 2.08                     | 0.53              |
| 22:BA:1432:G:O2'  | 22:BA:1433:A:H5'   | 2.09                     | 0.53              |
| 22:BA:480:A:H2'   | 22:BA:481:G:OP1    | 2.08                     | 0.53              |
| 22:BA:544:C:H5'   | 22:BA:545:U:OP2    | 2.08                     | 0.53              |
| 27:BF:121:SER:HB2 | 27:BF:128:TYR:CE1  | 2.44                     | 0.53              |
| 29:BH:147:VAL:CG1 | 29:BH:149:GLU:HG3  | 2.37                     | 0.53              |
| 38:BQ:58:ARG:O    | 38:BQ:62:ILE:HG13  | 2.09                     | 0.53              |
| 40:BS:4:ILE:HG12  | 40:BS:106:VAL:HG22 | 1.90                     | 0.53              |
| 1:CA:1388:C:C2    | 1:CA:1389:C:C5     | 2.97                     | 0.53              |
| 1:CA:31:G:C5      | 1:CA:306:A:H1'     | 2.44                     | 0.53              |
| 1:CA:451:A:H4'    | 1:CA:452:A:O4'     | 2.08                     | 0.53              |
| 1:CA:991:U:N3     | 1:CA:1212:U:O4'    | 2.42                     | 0.53              |
| 1:CA:1302:C:C4    | 13:CM:17:ILE:CD1   | 2.92                     | 0.53              |
| 22:DA:2044:C:N3   | 22:DA:2045:C:C5    | 2.77                     | 0.53              |
| 22:DA:2119:A:C6   | 22:DA:2170:A:C5    | 2.96                     | 0.53              |
| 22:DA:2146:C:C4'  | 22:DA:2147:A:OP1   | 2.55                     | 0.53              |
| 22:DA:2307:G:H4'  | 22:DA:2308:G:O5'   | 2.08                     | 0.53              |
| 22:DA:511:U:O4    | 22:DA:512:G:N1     | 2.41                     | 0.53              |
| 22:DA:613:A:O2'   | 22:DA:614:A:P      | 2.66                     | 0.53              |
| 22:DA:864:G:O6    | 22:DA:865:C:N4     | 2.42                     | 0.53              |
| 23:DB:11:C:C5     | 23:DB:12:C:C5      | 2.97                     | 0.53              |
| 23:DB:25:U:C4     | 23:DB:26:C:C4      | 2.96                     | 0.53              |
| 24:DC:240:PHE:CE1 | 24:DC:242:LYS:O    | 2.62                     | 0.53              |
| 29:DH:103:VAL:HA  | 29:DH:106:ALA:HB3  | 1.89                     | 0.53              |
| 29:DH:37:VAL:CG2  | 29:DH:38:PRO:HD2   | 2.39                     | 0.53              |
| 33:DL:56:PRO:HD2  | 33:DL:59:ARG:HB2   | 1.91                     | 0.53              |
| 1:AA:1076:U:O2    | 1:AA:1082:A:C2     | 2.62                     | 0.53              |
| 1:AA:1355:G:O2'   | 1:AA:1356:G:H5'    | 2.09                     | 0.53              |
| 1:AA:39:G:C2      | 1:AA:40:C:C6       | 2.97                     | 0.53              |
| 1:AA:901:A:N7     | 1:AA:902:G:H1'     | 2.24                     | 0.53              |
| 3:AC:148:GLY:HA3  | 3:AC:172:ARG:O     | 2.09                     | 0.53              |
| 4:AD:203:LEU:HD23 | 4:AD:204:TYR:CE2   | 2.44                     | 0.53              |
| 6:AF:85:ILE:O     | 6:AF:86:ARG:HG2    | 2.09                     | 0.53              |
| 1:AA:1373:G:H5''  | 7:AG:36:LYS:HB2    | 1.91                     | 0.53              |
| 9:AI:58:VAL:HG12  | 9:AI:58:VAL:O      | 2.08                     | 0.53              |
| 9:AI:80:ARG:NH1   | 9:AI:103:PHE:CD1   | 2.77                     | 0.53              |
| 22:BA:1713:A:C2   | 22:BA:1716:U:C6    | 2.96                     | 0.53              |
| 22:BA:1734:G:C4   | 22:BA:1735:A:C8    | 2.95                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:BA:1923:U:C2'   | 22:BA:1924:C:C5'   | 2.86                     | 0.53              |
| 26:BE:149:ILE:HD11 | 26:BE:172:ALA:HA   | 1.89                     | 0.53              |
| 35:BN:32:GLU:HA    | 35:BN:115:LEU:HD12 | 1.91                     | 0.53              |
| 38:BQ:89:GLU:H     | 39:BR:49:ILE:CD1   | 2.22                     | 0.53              |
| 39:BR:59:ILE:HG12  | 39:BR:101:ILE:HD12 | 1.90                     | 0.53              |
| 40:BS:1:MET:N      | 40:BS:109:ASP:OD1  | 2.41                     | 0.53              |
| 41:BT:16:VAL:O     | 41:BT:17:SER:HB3   | 2.09                     | 0.53              |
| 1:CA:350:G:C6      | 1:CA:351:G:C6      | 2.96                     | 0.53              |
| 1:CA:892:A:O2'     | 1:CA:1415:G:H4'    | 2.09                     | 0.53              |
| 7:CG:65:ALA:O      | 7:CG:127:ALA:HB1   | 2.09                     | 0.53              |
| 9:CI:84:THR:HG21   | 9:CI:103:PHE:HB3   | 1.91                     | 0.53              |
| 12:CL:28:PRO:HB2   | 12:CL:29:GLN:OE1   | 2.08                     | 0.53              |
| 22:DA:1695:G:H3'   | 22:DA:1695:G:N3    | 2.24                     | 0.53              |
| 22:DA:1874:C:H3'   | 22:DA:1875:G:C8    | 2.44                     | 0.53              |
| 22:DA:563:A:C4     | 22:DA:2018:G:C2    | 2.97                     | 0.53              |
| 22:DA:1938:A:C6    | 22:DA:2590:A:H1'   | 2.43                     | 0.53              |
| 22:DA:513:A:C2     | 22:DA:514:A:C5     | 2.96                     | 0.53              |
| 32:DK:66:LYS:NZ    | 32:DK:79:PHE:O     | 2.34                     | 0.53              |
| 1:AA:1425:U:O2'    | 1:AA:1426:G:H5'    | 2.08                     | 0.53              |
| 1:AA:269:C:H2'     | 1:AA:270:A:C8      | 2.44                     | 0.53              |
| 1:AA:858:G:O2'     | 1:AA:859:G:H5'     | 2.08                     | 0.53              |
| 2:AB:126:PHE:N     | 2:AB:126:PHE:HD2   | 2.07                     | 0.53              |
| 2:AB:219:ALA:O     | 2:AB:220:THR:CB    | 2.56                     | 0.53              |
| 3:AC:92:ALA:HB2    | 3:AC:99:ALA:HB3    | 1.91                     | 0.53              |
| 8:AH:10:MET:O      | 8:AH:12:THR:N      | 2.42                     | 0.53              |
| 8:AH:25:VAL:HG12   | 8:AH:61:LEU:HB2    | 1.90                     | 0.53              |
| 9:AI:30:ILE:HD11   | 9:AI:38:TYR:CD2    | 2.43                     | 0.53              |
| 22:BA:1319:C:H2'   | 22:BA:1320:C:H5'   | 1.91                     | 0.53              |
| 22:BA:1667:G:O2'   | 22:BA:1991:U:O4    | 2.17                     | 0.53              |
| 22:BA:2514:U:H2'   | 22:BA:2515:C:C6    | 2.44                     | 0.53              |
| 22:BA:2673:G:C2    | 22:BA:2674:G:C8    | 2.97                     | 0.53              |
| 22:BA:2685:G:OP1   | 32:BK:78:ARG:NH2   | 2.39                     | 0.53              |
| 22:BA:280:U:H2'    | 22:BA:281:C:O4'    | 2.08                     | 0.53              |
| 22:BA:846:U:O2'    | 22:BA:847:U:OP2    | 2.27                     | 0.53              |
| 30:BI:127:ARG:HA   | 30:BI:130:GLU:CG   | 2.38                     | 0.53              |
| 39:BR:16:GLU:OE1   | 39:BR:100:GLY:HA2  | 2.09                     | 0.53              |
| 1:CA:1053:G:O5'    | 1:CA:1054:C:H3'    | 2.08                     | 0.53              |
| 1:CA:1151:A:H1'    | 1:CA:1152:A:C8     | 2.43                     | 0.53              |
| 1:CA:1461:G:H2'    | 1:CA:1462:C:O4'    | 2.08                     | 0.53              |
| 1:CA:1483:A:N1     | 22:DA:1959:G:O2'   | 2.41                     | 0.53              |
| 1:CA:1417:G:N2     | 1:CA:1484:C:C4     | 2.76                     | 0.53              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CA:891:U:C5     | 1:CA:906:A:C2     | 2.97                     | 0.53              |
| 1:CA:1228:C:H5'   | 13:CM:113:ARG:HB2 | 1.91                     | 0.53              |
| 13:CM:20:THR:O    | 13:CM:20:THR:HG22 | 2.09                     | 0.53              |
| 22:DA:1099:G:N7   | 22:DA:1100:C:N4   | 2.57                     | 0.53              |
| 22:DA:1120:G:C6   | 22:DA:1121:C:C4   | 2.97                     | 0.53              |
| 22:DA:1027:A:N6   | 22:DA:1126:A:N3   | 2.57                     | 0.53              |
| 22:DA:1544:A:C6   | 22:DA:1545:A:C6   | 2.97                     | 0.53              |
| 22:DA:176:A:N7    | 22:DA:177:G:C6    | 2.77                     | 0.53              |
| 22:DA:1907:G:C2   | 22:DA:1924:C:O2   | 2.61                     | 0.53              |
| 22:DA:2162:G:H4'  | 22:DA:2163:A:OP1  | 2.08                     | 0.53              |
| 22:DA:2520:C:HO2' | 22:DA:2565:A:HO2' | 1.57                     | 0.53              |
| 22:DA:2656:U:OP2  | 22:DA:2664:G:N1   | 2.42                     | 0.53              |
| 22:DA:2820:A:C8   | 25:DD:196:ALA:CB  | 2.92                     | 0.53              |
| 22:DA:294:A:C6    | 22:DA:345:A:C4    | 2.97                     | 0.53              |
| 22:DA:640:C:C4    | 22:DA:641:U:C5    | 2.97                     | 0.53              |
| 22:DA:848:C:H2'   | 22:DA:849:A:C8    | 2.44                     | 0.53              |
| 28:DG:67:THR:O    | 28:DG:71:LEU:N    | 2.42                     | 0.53              |
| 30:DI:18:ALA:O    | 30:DI:19:ASN:CB   | 2.56                     | 0.53              |
| 36:DO:100:HIS:CG  | 36:DO:101:GLY:N   | 2.77                     | 0.53              |
| 42:DU:98:SER:O    | 42:DU:99:ASN:HB3  | 2.07                     | 0.53              |
| 1:AA:1508:A:H2'   | 1:AA:1509:C:O4'   | 2.09                     | 0.53              |
| 1:AA:33:A:H2'     | 1:AA:34:C:C6      | 2.44                     | 0.53              |
| 1:AA:834:U:C4     | 1:AA:835:U:C4     | 2.97                     | 0.53              |
| 3:AC:12:LEU:O     | 3:AC:14:ILE:N     | 2.42                     | 0.53              |
| 8:AH:25:VAL:CG1   | 8:AH:25:VAL:O     | 2.57                     | 0.53              |
| 9:AI:58:VAL:O     | 9:AI:59:GLU:CB    | 2.57                     | 0.53              |
| 15:AO:35:GLN:HB3  | 15:AO:59:MET:CE   | 2.39                     | 0.53              |
| 17:AQ:82:ALA:O    | 17:AQ:83:VAL:O    | 2.27                     | 0.53              |
| 22:BA:1289:C:O2'  | 22:BA:1330:C:H4'  | 2.09                     | 0.53              |
| 22:BA:1587:G:C4   | 22:BA:1588:G:C8   | 2.97                     | 0.53              |
| 22:BA:1747:U:H2'  | 22:BA:1748:C:C6   | 2.44                     | 0.53              |
| 22:BA:2314:A:O2'  | 22:BA:2315:G:H5'  | 2.09                     | 0.53              |
| 22:BA:475:C:C5    | 22:BA:481:G:O6    | 2.61                     | 0.53              |
| 29:BH:27:ARG:NH2  | 45:BX:60:ASP:CG   | 2.62                     | 0.53              |
| 37:BP:106:LYS:O   | 37:BP:109:ARG:HD3 | 2.09                     | 0.53              |
| 39:BR:51:VAL:HB   | 39:BR:52:PRO:CD   | 2.39                     | 0.53              |
| 1:CA:1161:C:O2    | 1:CA:1176:A:C2    | 2.62                     | 0.53              |
| 1:CA:223:A:H2'    | 1:CA:224:U:C6     | 2.45                     | 0.53              |
| 1:CA:106:C:O2     | 1:CA:379:C:H4'    | 2.09                     | 0.53              |
| 1:CA:619:U:H3     | 4:CD:131:ASN:HB3  | 1.74                     | 0.53              |
| 22:DA:1438:U:C5   | 22:DA:1552:A:N1   | 2.76                     | 0.53              |

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| Atom-1            | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 22:DA:1779:U:C5   | 22:DA:1784:A:N7     | 2.76                     | 0.53              |
| 22:DA:858:G:O2'   | 22:DA:2268:A:N3     | 2.23                     | 0.53              |
| 22:DA:324:A:C2    | 22:DA:325:G:H1'     | 2.44                     | 0.53              |
| 22:DA:370:G:O2'   | 22:DA:424:G:OP1     | 2.22                     | 0.53              |
| 24:DC:62:TYR:CE1  | 24:DC:63:ARG:O      | 2.62                     | 0.53              |
| 22:DA:600:G:H1'   | 26:DE:100:MET:CG    | 2.39                     | 0.53              |
| 27:DF:33:LYS:HD3  | 27:DF:92:ARG:NH1    | 2.24                     | 0.53              |
| 28:DG:11:VAL:O    | 28:DG:48:ASN:ND2    | 2.42                     | 0.53              |
| 30:DI:33:VAL:HG13 | 30:DI:67:PHE:CZ     | 2.44                     | 0.53              |
| 30:DI:8:TYR:HA    | 30:DI:59:ILE:HB     | 1.91                     | 0.53              |
| 37:DP:91:ALA:HB2  | 37:DP:113:ARG:HG3   | 1.91                     | 0.53              |
| 1:AA:1010:U:H2'   | 1:AA:1011:C:C6      | 2.44                     | 0.52              |
| 1:AA:109:A:C6     | 1:AA:326:G:C6       | 2.96                     | 0.52              |
| 1:AA:1157:A:C6    | 1:AA:1180:A:C5      | 2.98                     | 0.52              |
| 1:AA:374:A:H5''   | 1:AA:452:A:C2       | 2.43                     | 0.52              |
| 1:AA:57:G:C5      | 1:AA:58:C:C4        | 2.96                     | 0.52              |
| 5:AE:56:VAL:N     | 5:AE:57:PRO:HD2     | 2.24                     | 0.52              |
| 10:AJ:80:THR:O    | 10:AJ:83:THR:N      | 2.41                     | 0.52              |
| 12:AL:117:TYR:O   | 12:AL:119:VAL:HG23  | 2.09                     | 0.52              |
| 13:AM:16:VAL:CG2  | 13:AM:41:GLU:HB2    | 2.38                     | 0.52              |
| 49:B1:14:SER:HB3  | 49:B1:48:ILE:O      | 2.09                     | 0.52              |
| 53:B5:83:LYS:HB3  | 53:B5:87:ALA:HB3    | 1.90                     | 0.52              |
| 22:BA:1179:G:O6   | 22:BA:1180:U:N3     | 2.43                     | 0.52              |
| 22:BA:1346:G:O2'  | 22:BA:1347:A:H5'    | 2.10                     | 0.52              |
| 22:BA:1467:U:C4   | 22:BA:1546:G:C2     | 2.98                     | 0.52              |
| 22:BA:1916:A:OP2  | 22:BA:1917:U:OP2    | 2.27                     | 0.52              |
| 22:BA:2000:C:O2'  | 22:BA:2001:C:H5'    | 2.09                     | 0.52              |
| 22:BA:244:A:C2    | 22:BA:255:A:C4      | 2.97                     | 0.52              |
| 22:BA:2593:U:C2'  | 22:BA:2594:C:O5'    | 2.57                     | 0.52              |
| 22:BA:2061:G:C2   | 55:BA:3001:DOL:HC22 | 2.44                     | 0.52              |
| 22:BA:287:G:C2    | 22:BA:354:A:C2      | 2.97                     | 0.52              |
| 22:BA:580:U:H2'   | 22:BA:581:C:H6      | 1.73                     | 0.52              |
| 35:BN:14:SER:HA   | 35:BN:17:ARG:NH1    | 2.24                     | 0.52              |
| 37:BP:31:TRP:CZ2  | 37:BP:40:LEU:CD1    | 2.92                     | 0.52              |
| 22:BA:929:U:H1'   | 47:BZ:26:GLY:O      | 2.10                     | 0.52              |
| 1:CA:119:A:H4'    | 1:CA:120:A:O5'      | 2.09                     | 0.52              |
| 5:CE:153:VAL:O    | 5:CE:157:ARG:N      | 2.42                     | 0.52              |
| 5:CE:96:MET:HE3   | 5:CE:111:MET:HE3    | 1.91                     | 0.52              |
| 7:CG:68:ASN:O     | 7:CG:138:ARG:NH2    | 2.42                     | 0.52              |
| 12:CL:90:LEU:CB   | 12:CL:93:VAL:CG2    | 2.87                     | 0.52              |
| 13:CM:20:THR:HG23 | 13:CM:26:GLY:O      | 2.09                     | 0.52              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 20:CT:83:ILE:O     | 20:CT:87:ALA:HB3  | 2.09                     | 0.52              |
| 22:DA:1308:A:H2'   | 22:DA:1309:G:O4'  | 2.09                     | 0.52              |
| 22:DA:1288:G:C4    | 22:DA:1327:A:C2   | 2.98                     | 0.52              |
| 22:DA:1410:G:N1    | 22:DA:1411:U:O4   | 2.42                     | 0.52              |
| 22:DA:2031:A:C6    | 22:DA:2498:C:H1'  | 2.44                     | 0.52              |
| 22:DA:2575:C:H2'   | 22:DA:2578:G:O6   | 2.09                     | 0.52              |
| 22:DA:9:G:C6       | 22:DA:2629:U:C5   | 2.98                     | 0.52              |
| 22:DA:450:G:H2'    | 22:DA:451:U:H5''  | 1.90                     | 0.52              |
| 25:DD:208:LYS:O    | 25:DD:209:ALA:HB2 | 2.08                     | 0.52              |
| 27:DF:108:VAL:HG11 | 27:DF:176:PRO:CG  | 2.39                     | 0.52              |
| 46:DY:36:GLN:O     | 46:DY:37:LEU:C    | 2.48                     | 0.52              |
| 1:AA:1028:C:O2     | 1:AA:1034:G:C6    | 2.62                     | 0.52              |
| 1:AA:1130:A:C1'    | 1:AA:1146:A:C2    | 2.92                     | 0.52              |
| 1:AA:1145:A:HO2'   | 1:AA:1146:A:P     | 2.32                     | 0.52              |
| 1:AA:1277:C:HO2'   | 1:AA:1279:G:H8    | 1.54                     | 0.52              |
| 1:AA:173:U:C6      | 1:AA:197:A:C2     | 2.97                     | 0.52              |
| 1:AA:373:A:N3      | 1:AA:374:A:C8     | 2.78                     | 0.52              |
| 1:AA:568:G:N3      | 1:AA:569:C:C5     | 2.78                     | 0.52              |
| 4:AD:76:TYR:CD1    | 4:AD:76:TYR:C     | 2.83                     | 0.52              |
| 4:AD:84:GLY:O      | 4:AD:89:ASN:ND2   | 2.42                     | 0.52              |
| 8:AH:111:MET:HE2   | 8:AH:116:ALA:N    | 2.23                     | 0.52              |
| 22:BA:1384:A:H1'   | 22:BA:1405:U:H1'  | 1.91                     | 0.52              |
| 22:BA:1754:A:C6    | 22:BA:1755:A:C6   | 2.97                     | 0.52              |
| 22:BA:1857:G:C2    | 22:BA:1884:G:N3   | 2.77                     | 0.52              |
| 22:BA:744:U:P      | 57:BA:3655:HOH:O  | 2.67                     | 0.52              |
| 22:BA:768:G:C5     | 22:BA:769:U:C5    | 2.97                     | 0.52              |
| 22:BA:2314:A:OP1   | 27:BF:88:LYS:NZ   | 2.42                     | 0.52              |
| 29:BH:77:THR:HA    | 29:BH:143:ILE:O   | 2.09                     | 0.52              |
| 39:BR:52:PRO:O     | 39:BR:53:PHE:O    | 2.27                     | 0.52              |
| 41:BT:88:LYS:O     | 41:BT:89:GLU:HG2  | 2.09                     | 0.52              |
| 43:BV:48:MET:O     | 43:BV:51:GLN:HG3  | 2.09                     | 0.52              |
| 43:BV:8:VAL:HG23   | 43:BV:9:ARG:N     | 2.24                     | 0.52              |
| 1:CA:1068:G:C2'    | 1:CA:1069:C:H5'   | 2.38                     | 0.52              |
| 1:CA:718:A:C8      | 1:CA:719:C:C6     | 2.97                     | 0.52              |
| 4:CD:148:LYS:O     | 4:CD:149:ALA:HB3  | 2.07                     | 0.52              |
| 7:CG:46:ALA:HA     | 7:CG:121:ALA:HB2  | 1.92                     | 0.52              |
| 22:DA:1009:A:O2'   | 22:DA:1153:C:H4'  | 2.09                     | 0.52              |
| 22:DA:1071:G:O2'   | 22:DA:1072:C:O4'  | 2.21                     | 0.52              |
| 22:DA:1127:A:C3'   | 22:DA:1128:G:H5'' | 2.38                     | 0.52              |
| 22:DA:971:G:O2'    | 22:DA:983:A:N3    | 2.41                     | 0.52              |
| 29:DH:31:VAL:CB    | 29:DH:32:PRO:CD   | 2.86                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 29:DH:40:THR:O    | 29:DH:41:LYS:C    | 2.48                     | 0.52              |
| 35:DN:58:ASP:HA   | 35:DN:80:PHE:CD1  | 2.44                     | 0.52              |
| 1:AA:1108:G:H5'   | 3:AC:176:HIS:ND1  | 2.24                     | 0.52              |
| 1:AA:683:G:N2     | 11:AK:40:ASN:HA   | 2.24                     | 0.52              |
| 1:AA:76:G:H2'     | 1:AA:76:G:N3      | 2.23                     | 0.52              |
| 1:AA:855:U:N3     | 1:AA:856:C:C5     | 2.78                     | 0.52              |
| 2:AB:126:PHE:N    | 2:AB:126:PHE:CD2  | 2.76                     | 0.52              |
| 1:AA:1342:C:O2'   | 9:AI:126:GLN:HG3  | 2.09                     | 0.52              |
| 9:AI:45:ARG:HG2   | 9:AI:46:MET:SD    | 2.49                     | 0.52              |
| 10:AJ:36:VAL:HA   | 10:AJ:76:ILE:HA   | 1.90                     | 0.52              |
| 22:BA:1083:U:O2   | 22:BA:1085:A:C8   | 2.62                     | 0.52              |
| 22:BA:1508:A:O2'  | 22:BA:1509:A:O4'  | 2.25                     | 0.52              |
| 22:BA:2590:A:C2   | 22:BA:2605:U:C2   | 2.98                     | 0.52              |
| 22:BA:362:A:C8    | 22:BA:362:A:OP2   | 2.62                     | 0.52              |
| 22:BA:479:A:N3    | 22:BA:481:G:H5''  | 2.25                     | 0.52              |
| 23:BB:37:C:C5     | 23:BB:38:C:C4     | 2.98                     | 0.52              |
| 26:BE:91:ASP:OD1  | 26:BE:91:ASP:C    | 2.48                     | 0.52              |
| 45:BX:3:ARG:CD    | 45:BX:30:LEU:HD13 | 2.39                     | 0.52              |
| 1:CA:978:A:O2'    | 1:CA:1322:C:C5    | 2.63                     | 0.52              |
| 1:CA:718:A:C5'    | 11:CK:119:ASN:ND2 | 2.73                     | 0.52              |
| 1:CA:669:G:N2     | 1:CA:738:C:C2     | 2.77                     | 0.52              |
| 3:CC:130:PHE:CZ   | 3:CC:131:ARG:CD   | 2.92                     | 0.52              |
| 4:CD:3:ARG:HD2    | 4:CD:115:ARG:NE   | 2.25                     | 0.52              |
| 6:CF:93:LYS:O     | 6:CF:93:LYS:HG2   | 2.09                     | 0.52              |
| 9:CI:120:LYS:CG   | 9:CI:123:ARG:HB3  | 2.38                     | 0.52              |
| 14:CN:52:PRO:O    | 14:CN:53:ARG:HB3  | 2.09                     | 0.52              |
| 22:DA:1786:A:H1'  | 22:DA:1938:A:N6   | 2.24                     | 0.52              |
| 22:DA:2111:U:C4   | 22:DA:2147:A:C2   | 2.97                     | 0.52              |
| 22:DA:237:C:N3    | 22:DA:238:C:C5    | 2.77                     | 0.52              |
| 22:DA:2562:U:C2'  | 22:DA:2563:U:H5'  | 2.40                     | 0.52              |
| 22:DA:2586:U:C6   | 22:DA:2587:A:C8   | 2.98                     | 0.52              |
| 22:DA:32:C:H5''   | 22:DA:33:C:OP2    | 2.10                     | 0.52              |
| 22:DA:27:G:N2     | 22:DA:512:G:H1'   | 2.23                     | 0.52              |
| 25:DD:183:GLU:OE1 | 25:DD:183:GLU:N   | 2.42                     | 0.52              |
| 29:DH:72:ILE:HG22 | 29:DH:72:ILE:O    | 2.09                     | 0.52              |
| 36:DO:79:ALA:O    | 36:DO:83:LEU:HG   | 2.08                     | 0.52              |
| 1:AA:1311:A:C2    | 1:AA:1327:C:N3    | 2.77                     | 0.52              |
| 1:AA:1337:G:C5'   | 1:AA:1338:G:OP1   | 2.56                     | 0.52              |
| 1:AA:602:A:C2     | 1:AA:603:U:O2     | 2.62                     | 0.52              |
| 1:AA:832:G:N3     | 1:AA:833:G:C8     | 2.78                     | 0.52              |
| 15:AO:4:SER:O     | 15:AO:8:THR:OG1   | 2.26                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:AK:126:LYS:O   | 21:AU:34:ARG:NE   | 2.42                     | 0.52              |
| 33:BL:48:ARG:HD2  | 51:B3:60:ALA:O    | 2.10                     | 0.52              |
| 53:B5:19:LYS:HG3  | 53:B5:23:ILE:HG12 | 1.92                     | 0.52              |
| 22:BA:686:U:H4'   | 22:BA:687:C:OP2   | 2.09                     | 0.52              |
| 42:BU:86:ARG:NH1  | 42:BU:100:SER:O   | 2.41                     | 0.52              |
| 1:CA:1055:A:C6    | 1:CA:1206:G:C5    | 2.98                     | 0.52              |
| 1:CA:632:U:H2'    | 1:CA:632:U:O2     | 2.08                     | 0.52              |
| 1:CA:747:A:C6     | 1:CA:748:G:C6     | 2.97                     | 0.52              |
| 2:CB:167:ASP:OD2  | 2:CB:191:SER:HA   | 2.10                     | 0.52              |
| 16:CP:28:ARG:CG   | 16:CP:29:ASN:OD1  | 2.56                     | 0.52              |
| 22:DA:2372:U:O4'  | 49:D1:46:HIS:ND1  | 2.42                     | 0.52              |
| 22:DA:1390:U:C2'  | 22:DA:1391:U:H5'  | 2.40                     | 0.52              |
| 22:DA:307:G:N1    | 22:DA:310:A:OP2   | 2.43                     | 0.52              |
| 22:DA:498:G:C2    | 22:DA:499:U:C5    | 2.97                     | 0.52              |
| 22:DA:830:G:C2    | 22:DA:2448:A:N7   | 2.77                     | 0.52              |
| 28:DG:19:ILE:O    | 28:DG:21:GLY:N    | 2.43                     | 0.52              |
| 30:DI:80:LEU:HD23 | 30:DI:84:ALA:HB2  | 1.91                     | 0.52              |
| 34:DM:31:PHE:CZ   | 34:DM:110:GLU:HA  | 2.45                     | 0.52              |
| 36:DO:33:ARG:O    | 36:DO:34:HIS:CD2  | 2.62                     | 0.52              |
| 40:DS:28:LYS:O    | 40:DS:29:VAL:C    | 2.48                     | 0.52              |
| 1:AA:1076:U:C2    | 1:AA:1082:A:C2    | 2.97                     | 0.52              |
| 1:AA:1167:A:N7    | 1:AA:1169:A:C5    | 2.78                     | 0.52              |
| 1:AA:1260:G:OP1   | 1:AA:1284:C:O2'   | 2.27                     | 0.52              |
| 1:AA:262:A:H2'    | 1:AA:263:A:C8     | 2.43                     | 0.52              |
| 1:AA:268:U:H2'    | 1:AA:269:C:C6     | 2.44                     | 0.52              |
| 1:AA:542:G:OP1    | 4:AD:10:LYS:HE2   | 2.10                     | 0.52              |
| 4:AD:51:TYR:CE2   | 4:AD:55:LEU:HD12  | 2.45                     | 0.52              |
| 5:AE:46:VAL:HG22  | 5:AE:118:ALA:HA   | 1.91                     | 0.52              |
| 6:AF:36:ILE:O     | 6:AF:36:ILE:HG23  | 2.09                     | 0.52              |
| 6:AF:3:HIS:O      | 6:AF:92:THR:HG23  | 2.09                     | 0.52              |
| 9:AI:52:LEU:HD13  | 9:AI:57:MET:HG3   | 1.91                     | 0.52              |
| 10:AJ:63:ASP:HB3  | 10:AJ:65:TYR:CE2  | 2.45                     | 0.52              |
| 20:AT:25:ARG:HG2  | 20:AT:29:ARG:NH1  | 2.23                     | 0.52              |
| 20:AT:29:ARG:O    | 20:AT:33:LYS:HG2  | 2.10                     | 0.52              |
| 22:BA:2055:C:H5'  | 22:BA:2056:G:O5'  | 2.10                     | 0.52              |
| 22:BA:2308:G:O6   | 22:BA:2311:A:C8   | 2.62                     | 0.52              |
| 22:BA:2747:G:O2'  | 28:BG:67:THR:HB   | 2.09                     | 0.52              |
| 22:BA:2771:C:H2'  | 22:BA:2772:C:C6   | 2.45                     | 0.52              |
| 22:BA:573:U:O2'   | 22:BA:574:A:H3'   | 2.09                     | 0.52              |
| 22:BA:998:C:C2'   | 22:BA:999:U:O5'   | 2.58                     | 0.52              |
| 26:BE:15:SER:N    | 26:BE:197:GLU:OE2 | 2.42                     | 0.52              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 28:BG:121:ILE:CD1 | 28:BG:141:ILE:HG22 | 2.40                     | 0.52              |
| 29:BH:51:ARG:NH1  | 29:BH:55:GLU:OE1   | 2.43                     | 0.52              |
| 37:BP:31:TRP:CE2  | 37:BP:40:LEU:HD11  | 2.45                     | 0.52              |
| 39:BR:49:ILE:CB   | 39:BR:52:PRO:O     | 2.57                     | 0.52              |
| 39:BR:74:ILE:CD1  | 39:BR:74:ILE:N     | 2.71                     | 0.52              |
| 1:CA:1232:U:OP1   | 9:CI:126:GLN:HG2   | 2.10                     | 0.52              |
| 1:CA:32:A:H2'     | 1:CA:33:A:C8       | 2.44                     | 0.52              |
| 1:CA:519:C:H2'    | 1:CA:520:A:O4'     | 2.10                     | 0.52              |
| 1:CA:644:U:H2'    | 1:CA:645:G:O4'     | 2.10                     | 0.52              |
| 1:CA:73:C:C2      | 1:CA:74:A:C8       | 2.98                     | 0.52              |
| 17:CQ:48:ASP:N    | 17:CQ:48:ASP:OD2   | 2.41                     | 0.52              |
| 22:DA:2615:U:C4   | 48:D0:3:VAL:O      | 2.62                     | 0.52              |
| 22:DA:1567:G:C8   | 24:DC:83:TYR:CE1   | 2.98                     | 0.52              |
| 22:DA:1645:G:H4'  | 22:DA:1646:C:C6    | 2.44                     | 0.52              |
| 22:DA:1678:A:C5   | 22:DA:1679:A:C8    | 2.97                     | 0.52              |
| 22:DA:1783:A:C6   | 22:DA:2587:A:C2    | 2.97                     | 0.52              |
| 22:DA:1799:G:N1   | 22:DA:1819:A:OP2   | 2.40                     | 0.52              |
| 22:DA:2016:U:O2   | 48:D0:4:GLN:NE2    | 2.43                     | 0.52              |
| 22:DA:2060:A:O4'  | 22:DA:2502:G:H1'   | 2.10                     | 0.52              |
| 22:DA:2341:G:C5   | 22:DA:2342:C:C4    | 2.98                     | 0.52              |
| 22:DA:2772:C:H5'  | 25:DD:173:GLN:NE2  | 2.25                     | 0.52              |
| 22:DA:2842:G:C2   | 22:DA:2843:G:H1'   | 2.45                     | 0.52              |
| 22:DA:1800:C:OP1  | 24:DC:258:ARG:NH2  | 2.42                     | 0.52              |
| 29:DH:34:GLY:O    | 29:DH:35:LYS:HD2   | 2.10                     | 0.52              |
| 33:DL:29:LYS:HG3  | 33:DL:30:THR:HG23  | 1.91                     | 0.52              |
| 34:DM:119:LEU:O   | 34:DM:119:LEU:HD13 | 2.10                     | 0.52              |
| 40:DS:63:GLY:O    | 40:DS:64:ALA:HB3   | 2.10                     | 0.52              |
| 1:AA:1014:A:H4'   | 19:AS:14:HIS:CE1   | 2.45                     | 0.52              |
| 1:AA:189:A:H2'    | 1:AA:190:A:O4'     | 2.10                     | 0.52              |
| 2:AB:20:THR:HA    | 2:AB:38:VAL:HA     | 1.90                     | 0.52              |
| 2:AB:81:LYS:HG3   | 2:AB:91:PHE:CZ     | 2.45                     | 0.52              |
| 4:AD:130:VAL:HG11 | 4:AD:135:TYR:CG    | 2.45                     | 0.52              |
| 5:AE:94:VAL:CG2   | 5:AE:111:MET:SD    | 2.98                     | 0.52              |
| 5:AE:104:GLY:HA3  | 5:AE:122:ASN:HA    | 1.91                     | 0.52              |
| 10:AJ:57:VAL:O    | 10:AJ:58:ASN:HB2   | 2.09                     | 0.52              |
| 20:AT:33:LYS:O    | 20:AT:34:LYS:C     | 2.48                     | 0.52              |
| 22:BA:852:U:H2'   | 22:BA:853:C:C6     | 2.44                     | 0.52              |
| 1:CA:1298:U:O2    | 1:CA:1298:U:C2'    | 2.57                     | 0.52              |
| 1:CA:151:A:H2'    | 1:CA:152:A:O4'     | 2.09                     | 0.52              |
| 1:CA:542:G:C2     | 1:CA:543:U:C5      | 2.98                     | 0.52              |
| 2:CB:91:PHE:CD2   | 2:CB:150:GLY:HA3   | 2.44                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:CD:22:LYS:O     | 4:CD:24:GLY:N     | 2.43                     | 0.52              |
| 7:CG:74:GLU:O     | 7:CG:88:PRO:HA    | 2.10                     | 0.52              |
| 15:CO:53:ARG:O    | 15:CO:56:LEU:HB3  | 2.09                     | 0.52              |
| 19:CS:15:LEU:HD13 | 19:CS:33:THR:HG21 | 1.92                     | 0.52              |
| 20:CT:32:ILE:HG12 | 20:CT:54:MET:HE3  | 1.90                     | 0.52              |
| 22:DA:1087:G:C2   | 22:DA:1089:A:C2   | 2.98                     | 0.52              |
| 22:DA:1101:U:C5   | 22:DA:1102:C:C5   | 2.97                     | 0.52              |
| 22:DA:1980:G:O2'  | 22:DA:1982:U:OP2  | 2.26                     | 0.52              |
| 22:DA:2258:C:H4'  | 22:DA:2259:U:OP2  | 2.10                     | 0.52              |
| 22:DA:2747:G:O6   | 22:DA:2755:C:H5'' | 2.09                     | 0.52              |
| 22:DA:481:G:C4    | 22:DA:507:A:C2    | 2.98                     | 0.52              |
| 22:DA:881:G:N1    | 22:DA:895:U:O2    | 2.42                     | 0.52              |
| 22:DA:2599:G:N7   | 24:DC:236:GLU:CB  | 2.73                     | 0.52              |
| 30:DI:114:ALA:O   | 30:DI:115:ALA:HB2 | 2.10                     | 0.52              |
| 32:DK:121:GLU:O   | 32:DK:122:VAL:O   | 2.28                     | 0.52              |
| 34:DM:124:LEU:N   | 34:DM:124:LEU:CD2 | 2.72                     | 0.52              |
| 22:DA:2870:C:H5'' | 35:DN:65:LEU:HD21 | 1.90                     | 0.52              |
| 37:DP:39:ARG:HA   | 37:DP:39:ARG:HE   | 1.73                     | 0.52              |
| 25:DD:15:PHE:CD2  | 37:DP:78:SER:HA   | 2.45                     | 0.52              |
| 1:AA:1070:U:C2    | 1:AA:1071:C:C5    | 2.98                     | 0.52              |
| 1:AA:887:G:H2'    | 1:AA:888:G:H5'    | 1.91                     | 0.52              |
| 2:AB:67:ILE:O     | 2:AB:68:LEU:CB    | 2.57                     | 0.52              |
| 4:AD:107:PHE:CD1  | 4:AD:145:ILE:CD1  | 2.93                     | 0.52              |
| 19:AS:64:ASP:HB3  | 27:BF:115:ARG:NH2 | 2.24                     | 0.52              |
| 20:AT:68:HIS:HB3  | 20:AT:69:LYS:NZ   | 2.25                     | 0.52              |
| 21:AU:17:ARG:NH1  | 21:AU:20:LYS:CG   | 2.73                     | 0.52              |
| 53:B5:65:LEU:HD21 | 53:B5:191:ARG:CB  | 2.39                     | 0.52              |
| 22:BA:1288:G:C5   | 22:BA:1327:A:C2   | 2.98                     | 0.52              |
| 22:BA:1923:U:HO2' | 22:BA:1924:C:C5'  | 2.22                     | 0.52              |
| 22:BA:790:U:O2'   | 22:BA:791:C:O5'   | 2.26                     | 0.52              |
| 24:BC:123:ALA:O   | 24:BC:125:LYS:N   | 2.43                     | 0.52              |
| 27:BF:36:LEU:HD22 | 27:BF:91:LEU:HD11 | 1.91                     | 0.52              |
| 29:BH:94:ILE:HD12 | 29:BH:98:ASP:HB3  | 1.92                     | 0.52              |
| 34:BM:78:LEU:N    | 34:BM:78:LEU:HD12 | 2.24                     | 0.52              |
| 35:BN:21:PHE:HB3  | 35:BN:47:VAL:HG21 | 1.92                     | 0.52              |
| 38:BQ:41:LYS:HG3  | 38:BQ:45:TYR:CE1  | 2.44                     | 0.52              |
| 46:BY:14:LEU:HA   | 46:BY:17:GLU:HB3  | 1.92                     | 0.52              |
| 1:CA:1296:C:H5''  | 1:CA:1297:G:OP2   | 2.09                     | 0.52              |
| 1:CA:1306:A:H1'   | 1:CA:1332:A:C5    | 2.45                     | 0.52              |
| 1:CA:421:U:O5'    | 1:CA:422:C:C5     | 2.62                     | 0.52              |
| 1:CA:484:G:N7     | 1:CA:486:U:H1'    | 2.24                     | 0.52              |

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| Atom-1             | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 1:CA:518:C:OP2     | 1:CA:530:G:H1'   | 2.08                     | 0.52              |
| 1:CA:71:A:C2       | 1:CA:72:A:C8     | 2.98                     | 0.52              |
| 2:CB:15:HIS:ND1    | 2:CB:15:HIS:C    | 2.63                     | 0.52              |
| 4:CD:46:PRO:O      | 4:CD:48:LEU:N    | 2.42                     | 0.52              |
| 11:CK:40:ASN:O     | 11:CK:41:ALA:HB3 | 2.10                     | 0.52              |
| 1:CA:553:A:O2'     | 12:CL:26:ALA:O   | 2.27                     | 0.52              |
| 16:CP:23:ASP:OD2   | 16:CP:25:ARG:CG  | 2.58                     | 0.52              |
| 20:CT:36:TYR:CD1   | 20:CT:36:TYR:C   | 2.83                     | 0.52              |
| 22:DA:1327:A:H2'   | 22:DA:1328:A:O4' | 2.10                     | 0.52              |
| 22:DA:1726:C:H2'   | 22:DA:1727:C:C6  | 2.45                     | 0.52              |
| 22:DA:1869:G:C2    | 22:DA:1873:G:N1  | 2.78                     | 0.52              |
| 22:DA:1875:G:O2'   | 22:DA:1876:A:OP2 | 2.28                     | 0.52              |
| 22:DA:1957:C:H5'   | 22:DA:1984:G:O2' | 2.09                     | 0.52              |
| 22:DA:2234:G:C5    | 22:DA:2235:G:C8  | 2.98                     | 0.52              |
| 22:DA:2301:C:C2    | 22:DA:2316:G:N2  | 2.77                     | 0.52              |
| 22:DA:2546:U:O4'   | 22:DA:2565:A:C2  | 2.62                     | 0.52              |
| 22:DA:2810:A:C8    | 22:DA:2811:G:C8  | 2.98                     | 0.52              |
| 22:DA:305:C:H1'    | 22:DA:313:G:N2   | 2.24                     | 0.52              |
| 22:DA:574:A:H4'    | 22:DA:575:A:C5'  | 2.39                     | 0.52              |
| 22:DA:621:A:C5     | 22:DA:622:G:H1'  | 2.44                     | 0.52              |
| 29:DH:34:GLY:O     | 29:DH:35:LYS:HB2 | 2.08                     | 0.52              |
| 33:DL:56:PRO:O     | 33:DL:60:ARG:CB  | 2.57                     | 0.52              |
| 37:DP:91:ALA:HB2   | 37:DP:113:ARG:HA | 1.90                     | 0.52              |
| 1:AA:1425:U:O2     | 1:AA:1476:A:C2   | 2.62                     | 0.52              |
| 1:AA:622:A:C8      | 1:AA:623:C:C6    | 2.98                     | 0.52              |
| 1:AA:80:A:C2       | 1:AA:90:C:N3     | 2.77                     | 0.52              |
| 1:AA:968:A:H4'     | 1:AA:969:A:OP2   | 2.10                     | 0.52              |
| 1:AA:980:C:C5      | 1:AA:981:U:C5    | 2.97                     | 0.52              |
| 1:AA:9:G:C6        | 1:AA:26:A:N6     | 2.78                     | 0.52              |
| 2:AB:75:ALA:O      | 2:AB:76:ALA:CB   | 2.58                     | 0.52              |
| 49:B1:6:ARG:HG2    | 49:B1:24:THR:HB  | 1.92                     | 0.52              |
| 22:BA:1142:A:C2    | 22:BA:1144:A:C1' | 2.92                     | 0.52              |
| 22:BA:1424:G:H2'   | 22:BA:1425:G:O4' | 2.10                     | 0.52              |
| 22:BA:2199:A:C8    | 22:BA:2200:C:C5  | 2.97                     | 0.52              |
| 22:BA:226:A:C6     | 22:BA:227:A:C6   | 2.97                     | 0.52              |
| 22:BA:264:C:O2'    | 22:BA:265:A:H2'  | 2.10                     | 0.52              |
| 22:BA:591:U:HO2'   | 51:B3:2:PRO:N    | 2.07                     | 0.52              |
| 22:BA:624:C:O2'    | 22:BA:657:U:H5'' | 2.09                     | 0.52              |
| 24:BC:141:VAL:HG13 | 24:BC:191:THR:O  | 2.10                     | 0.52              |
| 29:BH:2:GLN:O      | 29:BH:3:VAL:HG22 | 2.10                     | 0.52              |
| 32:BK:58:LEU:HD23  | 32:BK:59:LYS:O   | 2.10                     | 0.52              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 40:BS:36:LEU:HD13 | 40:BS:48:LYS:CA   | 2.40                     | 0.52              |
| 1:CA:1416:G:N2    | 1:CA:1485:U:H1'   | 2.24                     | 0.52              |
| 1:CA:643:C:H5'    | 8:CH:32:LEU:HD22  | 1.92                     | 0.52              |
| 2:CB:62:SER:HA    | 2:CB:224:GLY:HA3  | 1.91                     | 0.52              |
| 21:CU:14:VAL:C    | 21:CU:16:LEU:HG   | 2.29                     | 0.52              |
| 22:DA:1340:U:H4'  | 22:DA:1341:G:OP2  | 2.10                     | 0.52              |
| 22:DA:389:G:O4'   | 22:DA:2413:G:H5'  | 2.10                     | 0.52              |
| 22:DA:1782:U:O4   | 22:DA:2586:U:C5   | 2.62                     | 0.52              |
| 25:DD:86:GLU:HG3  | 25:DD:87:GLY:N    | 2.24                     | 0.52              |
| 29:DH:25:TYR:CZ   | 29:DH:30:LEU:HD21 | 2.45                     | 0.52              |
| 37:DP:113:ARG:O   | 37:DP:114:LEU:C   | 2.48                     | 0.52              |
| 40:DS:7:HIS:HB2   | 40:DS:50:VAL:HG21 | 1.92                     | 0.52              |
| 42:DU:41:LEU:HD12 | 42:DU:60:GLU:CG   | 2.40                     | 0.52              |
| 1:AA:1004:A:H2'   | 1:AA:1005:A:O4'   | 2.10                     | 0.52              |
| 1:AA:1080:A:O3'   | 5:AE:21:VAL:HG21  | 2.09                     | 0.52              |
| 1:AA:1327:C:C2'   | 1:AA:1328:C:H5'   | 2.40                     | 0.52              |
| 1:AA:1410:A:C4    | 1:AA:1491:G:N2    | 2.78                     | 0.52              |
| 2:AB:68:LEU:HD21  | 2:AB:92:VAL:HG23  | 1.92                     | 0.52              |
| 7:AG:42:ILE:HG21  | 7:AG:116:MET:HB3  | 1.92                     | 0.52              |
| 9:AI:50:GLN:C     | 9:AI:52:LEU:H     | 2.12                     | 0.52              |
| 49:B1:34:LEU:H    | 49:B1:52:ALA:CB   | 2.23                     | 0.52              |
| 22:BA:1020:A:C2   | 22:BA:1141:U:C2   | 2.98                     | 0.52              |
| 22:BA:1179:G:O6   | 22:BA:1180:U:C2   | 2.63                     | 0.52              |
| 22:BA:1820:U:O4   | 24:BC:198:ALA:HB1 | 2.09                     | 0.52              |
| 22:BA:2355:G:O3'  | 44:BW:24:LYS:NZ   | 2.43                     | 0.52              |
| 22:BA:2554:U:C4   | 22:BA:2555:U:O4   | 2.63                     | 0.52              |
| 22:BA:528:A:C8    | 22:BA:528:A:C3'   | 2.93                     | 0.52              |
| 39:BR:47:VAL:HG12 | 39:BR:54:VAL:HG21 | 1.92                     | 0.52              |
| 40:BS:17:VAL:HG12 | 40:BS:76:VAL:HG21 | 1.92                     | 0.52              |
| 47:BZ:8:THR:OG1   | 47:BZ:35:THR:OG1  | 2.28                     | 0.52              |
| 1:CA:154:U:O2     | 1:CA:168:G:N2     | 2.43                     | 0.52              |
| 1:CA:517:G:H5'    | 1:CA:519:C:O2     | 2.10                     | 0.52              |
| 1:CA:609:A:N7     | 1:CA:610:U:C5     | 2.78                     | 0.52              |
| 13:CM:10:PRO:O    | 13:CM:11:ASP:HB2  | 2.10                     | 0.52              |
| 22:DA:1858:A:C2   | 22:DA:1859:U:C2   | 2.98                     | 0.52              |
| 22:DA:228:C:N3    | 22:DA:418:C:O4'   | 2.43                     | 0.52              |
| 25:DD:140:HIS:CE1 | 57:DD:303:HOH:O   | 2.63                     | 0.52              |
| 26:DE:77:ILE:CG1  | 26:DE:77:ILE:O    | 2.57                     | 0.52              |
| 27:DF:121:SER:O   | 27:DF:123:ASP:N   | 2.43                     | 0.52              |
| 28:DG:87:LEU:HD12 | 28:DG:87:LEU:N    | 2.25                     | 0.52              |
| 29:DH:23:ALA:O    | 29:DH:27:ARG:N    | 2.38                     | 0.52              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 34:DM:135:VAL:O    | 34:DM:136:MET:CB    | 2.57                     | 0.52              |
| 36:DO:36:TYR:CD1   | 36:DO:36:TYR:N      | 2.77                     | 0.52              |
| 1:AA:1018:G:N2     | 1:AA:1019:A:C8      | 2.77                     | 0.52              |
| 1:AA:1135:U:H2'    | 1:AA:1136:C:O5'     | 2.10                     | 0.52              |
| 1:AA:1356:G:N2     | 1:AA:1357:A:C2      | 2.78                     | 0.52              |
| 1:AA:188:C:O2      | 1:AA:188:C:H2'      | 2.09                     | 0.52              |
| 17:AQ:6:ARG:O      | 17:AQ:7:THR:HG23    | 2.09                     | 0.52              |
| 49:B1:47:VAL:HG13  | 49:B1:48:ILE:N      | 2.24                     | 0.52              |
| 22:BA:1132:U:C3'   | 22:BA:1133:A:H5''   | 2.39                     | 0.52              |
| 22:BA:1721:G:O2'   | 22:BA:1739:A:N6     | 2.43                     | 0.52              |
| 22:BA:2534:A:H2'   | 22:BA:2535:G:O5'    | 2.10                     | 0.52              |
| 22:BA:2684:U:C4    | 22:BA:2685:G:N7     | 2.78                     | 0.52              |
| 22:BA:760:G:H2'    | 22:BA:761:A:O4'     | 2.09                     | 0.52              |
| 27:BF:108:VAL:HG12 | 27:BF:109:PRO:HD3   | 1.91                     | 0.52              |
| 23:BB:54:G:H21     | 27:BF:26:MET:CE     | 2.23                     | 0.52              |
| 33:BL:95:LEU:HD22  | 33:BL:100:ILE:CD1   | 2.39                     | 0.52              |
| 37:BP:75:GLN:O     | 37:BP:77:HIS:N      | 2.43                     | 0.52              |
| 39:BR:66:HIS:CE1   | 39:BR:94:THR:CG2    | 2.92                     | 0.52              |
| 45:BX:68:LEU:HD13  | 45:BX:78:TYR:CE1    | 2.45                     | 0.52              |
| 1:CA:34:C:H2'      | 1:CA:35:G:C8        | 2.45                     | 0.52              |
| 1:CA:885:G:O2'     | 1:CA:914:A:N1       | 2.32                     | 0.52              |
| 3:CC:111:LEU:CD1   | 3:CC:146:ALA:HB2    | 2.40                     | 0.52              |
| 3:CC:77:ILE:HA     | 3:CC:84:VAL:HG23    | 1.92                     | 0.52              |
| 5:CE:105:ILE:H     | 5:CE:122:ASN:C      | 2.13                     | 0.52              |
| 5:CE:153:VAL:HG23  | 5:CE:157:ARG:HB2    | 1.90                     | 0.52              |
| 17:CQ:15:ASP:OD1   | 17:CQ:54:GLY:HA2    | 2.10                     | 0.52              |
| 22:DA:1293:C:H2'   | 22:DA:1294:U:O4'    | 2.10                     | 0.52              |
| 22:DA:2091:C:C3'   | 22:DA:2092:U:H5''   | 2.38                     | 0.52              |
| 22:DA:2502:G:H5'   | 22:DA:2503:A:H5''   | 1.92                     | 0.52              |
| 22:DA:2819:G:H2'   | 22:DA:2821:A:N7     | 2.25                     | 0.52              |
| 22:DA:2061:G:C6    | 55:DA:3001:DOL:HC19 | 2.44                     | 0.52              |
| 22:DA:396:G:OP2    | 45:DX:10:LYS:HG2    | 2.09                     | 0.52              |
| 22:DA:582:A:N7     | 57:DA:3286:HOH:O    | 2.34                     | 0.52              |
| 22:DA:621:A:C6     | 22:DA:622:G:H1'     | 2.45                     | 0.52              |
| 31:DJ:117:ALA:HA   | 31:DJ:120:ARG:HD2   | 1.91                     | 0.52              |
| 39:DR:82:HIS:CG    | 39:DR:82:HIS:O      | 2.63                     | 0.52              |
| 40:DS:20:VAL:CG2   | 40:DS:39:THR:HG21   | 2.40                     | 0.52              |
| 42:DU:54:GLN:N     | 42:DU:55:PRO:HD3    | 2.25                     | 0.52              |
| 1:AA:1010:U:O2     | 1:AA:1019:A:N1      | 2.43                     | 0.51              |
| 1:AA:1201:A:H1'    | 1:AA:1202:U:OP2     | 2.10                     | 0.51              |
| 1:AA:1202:U:C4     | 1:AA:1203:C:C5      | 2.98                     | 0.51              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:AA:1343:G:H2'    | 1:AA:1344:C:C6    | 2.45                     | 0.51              |
| 1:AA:208:U:C6      | 1:AA:210:C:C4     | 2.99                     | 0.51              |
| 1:AA:560:A:C6      | 5:AE:128:TYR:CE1  | 2.98                     | 0.51              |
| 1:AA:685:G:N1      | 1:AA:686:U:O4     | 2.43                     | 0.51              |
| 3:AC:140:ASN:O     | 3:AC:141:ALA:HB2  | 2.11                     | 0.51              |
| 4:AD:60:LYS:NZ     | 4:AD:194:ASP:O    | 2.43                     | 0.51              |
| 9:AI:43:THR:O      | 9:AI:44:ALA:CB    | 2.57                     | 0.51              |
| 10:AJ:56:HIS:ND1   | 10:AJ:57:VAL:HG12 | 2.25                     | 0.51              |
| 12:AL:25:GLU:O     | 12:AL:26:ALA:C    | 2.48                     | 0.51              |
| 15:AO:63:ARG:CG    | 15:AO:67:LEU:CD1  | 2.88                     | 0.51              |
| 15:AO:89:ARG:NH1   | 22:BA:714:U:C5    | 2.78                     | 0.51              |
| 22:BA:1627:G:C2    | 22:BA:1628:G:C8   | 2.98                     | 0.51              |
| 22:BA:2553:G:N1    | 22:BA:2554:U:O2   | 2.43                     | 0.51              |
| 22:BA:988:A:OP2    | 47:BZ:12:SER:HB3  | 2.10                     | 0.51              |
| 30:BI:75:PRO:O     | 30:BI:79:LEU:HD12 | 2.10                     | 0.51              |
| 44:BW:56:ASP:OD1   | 44:BW:56:ASP:N    | 2.39                     | 0.51              |
| 1:CA:949:A:C2      | 1:CA:1233:G:N3    | 2.78                     | 0.51              |
| 1:CA:179:A:H2'     | 1:CA:180:U:C6     | 2.45                     | 0.51              |
| 1:CA:957:U:O2      | 1:CA:959:A:C8     | 2.62                     | 0.51              |
| 4:CD:192:SER:O     | 4:CD:193:ALA:HB3  | 2.10                     | 0.51              |
| 5:CE:157:ARG:HD3   | 5:CE:158:GLY:H    | 1.75                     | 0.51              |
| 1:CA:1060:U:C5'    | 10:CJ:53:ILE:HG23 | 2.41                     | 0.51              |
| 11:CK:77:TYR:N     | 11:CK:77:TYR:CD1  | 2.78                     | 0.51              |
| 11:CK:92:GLY:O     | 11:CK:93:ARG:C    | 2.49                     | 0.51              |
| 22:DA:1050:A:C2    | 22:DA:2751:G:C4   | 2.98                     | 0.51              |
| 22:DA:1362:C:H2'   | 22:DA:1363:C:H5'  | 1.91                     | 0.51              |
| 22:DA:1874:C:C4    | 22:DA:1875:G:C6   | 2.99                     | 0.51              |
| 22:DA:1906:G:OP1   | 22:DA:1930:G:C8   | 2.62                     | 0.51              |
| 22:DA:1649:G:O6    | 22:DA:2009:A:N6   | 2.43                     | 0.51              |
| 22:DA:2156:G:C6    | 22:DA:2157:G:C2   | 2.97                     | 0.51              |
| 22:DA:2283:C:C2    | 22:DA:2389:G:C2   | 2.98                     | 0.51              |
| 22:DA:294:A:N6     | 22:DA:345:A:C4    | 2.78                     | 0.51              |
| 22:DA:600:G:H1'    | 26:DE:100:MET:HG2 | 1.92                     | 0.51              |
| 22:DA:607:U:O4     | 22:DA:619:G:H2'   | 2.08                     | 0.51              |
| 22:DA:686:U:H6     | 22:DA:788:A:N1    | 2.08                     | 0.51              |
| 26:DE:149:ILE:HD12 | 26:DE:172:ALA:HA  | 1.92                     | 0.51              |
| 39:DR:49:ILE:HD12  | 39:DR:52:PRO:HA   | 1.92                     | 0.51              |
| 42:DU:82:ARG:O     | 42:DU:97:LYS:HB2  | 2.10                     | 0.51              |
| 42:DU:88:GLU:O     | 42:DU:89:ASP:CB   | 2.59                     | 0.51              |
| 1:AA:142:G:H3'     | 1:AA:143:A:C8     | 2.46                     | 0.51              |
| 1:AA:29:U:O2'      | 1:AA:30:U:H5'     | 2.10                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:AD:34:ILE:O      | 4:AD:34:ILE:HD13   | 2.11                     | 0.51              |
| 5:AE:136:VAL:O     | 5:AE:140:THR:HG23  | 2.10                     | 0.51              |
| 8:AH:125:ILE:O     | 8:AH:125:ILE:CG1   | 2.59                     | 0.51              |
| 20:AT:55:GLN:N     | 20:AT:56:PRO:HD2   | 2.25                     | 0.51              |
| 53:B5:191:ARG:O    | 53:B5:195:ARG:CB   | 2.57                     | 0.51              |
| 22:BA:1028:A:H61   | 22:BA:1125:G:H2'   | 1.76                     | 0.51              |
| 22:BA:1138:G:H5''  | 22:BA:1139:G:OP2   | 2.10                     | 0.51              |
| 22:BA:1429:G:O2'   | 22:BA:1430:G:H5'   | 2.10                     | 0.51              |
| 22:BA:1731:G:C6    | 22:BA:1733:G:C6    | 2.98                     | 0.51              |
| 22:BA:1935:G:C6    | 22:BA:1962:C:C6    | 2.98                     | 0.51              |
| 22:BA:2547:A:H2'   | 22:BA:2548:U:C6    | 2.45                     | 0.51              |
| 25:BD:140:HIS:CE1  | 57:BD:302:HOH:O    | 2.57                     | 0.51              |
| 29:BH:110:VAL:HG22 | 29:BH:114:GLU:HB2  | 1.90                     | 0.51              |
| 37:BP:91:ALA:HB2   | 37:BP:113:ARG:HA   | 1.93                     | 0.51              |
| 44:BW:56:ASP:O     | 44:BW:57:HIS:HB2   | 2.10                     | 0.51              |
| 46:BY:26:PHE:C     | 46:BY:26:PHE:CD1   | 2.83                     | 0.51              |
| 46:BY:45:GLN:O     | 46:BY:46:VAL:CB    | 2.58                     | 0.51              |
| 1:CA:1105:A:N3     | 1:CA:1106:G:C8     | 2.78                     | 0.51              |
| 1:CA:1157:A:H4'    | 1:CA:1158:C:O5'    | 2.10                     | 0.51              |
| 1:CA:1238:A:N3     | 1:CA:1241:G:O2'    | 2.35                     | 0.51              |
| 1:CA:575:G:C6      | 1:CA:821:G:C5      | 2.98                     | 0.51              |
| 19:CS:73:GLU:HB2   | 19:CS:74:PHE:CE1   | 2.45                     | 0.51              |
| 22:DA:1407:G:N2    | 22:DA:1596:A:N3    | 2.58                     | 0.51              |
| 22:DA:2651:C:O2'   | 22:DA:2652:C:H5'   | 2.10                     | 0.51              |
| 22:DA:2824:C:N4    | 22:DA:2825:G:C5    | 2.78                     | 0.51              |
| 22:DA:777:G:N7     | 22:DA:793:A:C2     | 2.79                     | 0.51              |
| 30:DI:86:ILE:HD13  | 30:DI:89:GLY:N     | 2.26                     | 0.51              |
| 35:DN:90:ARG:NH2   | 35:DN:116:VAL:HG11 | 2.25                     | 0.51              |
| 22:DA:483:A:H4'    | 42:DU:47:LYS:HA    | 1.92                     | 0.51              |
| 47:DZ:14:ILE:HG22  | 47:DZ:15:GLY:N     | 2.26                     | 0.51              |
| 1:AA:1253:G:N1     | 1:AA:1285:A:N6     | 2.58                     | 0.51              |
| 1:AA:1370:G:C5'    | 9:AI:111:VAL:HG21  | 2.40                     | 0.51              |
| 3:AC:87:LEU:O      | 3:AC:88:ARG:C      | 2.48                     | 0.51              |
| 16:AP:29:ASN:N     | 16:AP:29:ASN:OD1   | 2.43                     | 0.51              |
| 21:AU:12:PHE:CD2   | 21:AU:12:PHE:N     | 2.75                     | 0.51              |
| 11:AK:112:ASP:CB   | 21:AU:20:LYS:HD2   | 2.41                     | 0.51              |
| 22:BA:1313:U:H2'   | 22:BA:1610:A:C2    | 2.45                     | 0.51              |
| 22:BA:136:G:H2'    | 22:BA:137:U:C6     | 2.46                     | 0.51              |
| 22:BA:1394:U:P     | 57:BA:3410:HOH:O   | 2.68                     | 0.51              |
| 22:BA:1820:U:H4'   | 22:BA:1821:A:OP2   | 2.10                     | 0.51              |
| 22:BA:981:A:H5''   | 57:BA:3596:HOH:O   | 2.09                     | 0.51              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 33:BL:100:ILE:HG13 | 33:BL:100:ILE:O   | 2.10                     | 0.51              |
| 1:CA:1337:G:C5'    | 1:CA:1338:G:OP1   | 2.59                     | 0.51              |
| 1:CA:1537:U:C5     | 1:CA:1538:C:C4    | 2.98                     | 0.51              |
| 1:CA:583:A:C2      | 1:CA:759:A:C5     | 2.98                     | 0.51              |
| 2:CB:128:LYS:O     | 2:CB:129:LEU:HB2  | 2.09                     | 0.51              |
| 7:CG:25:LYS:O      | 7:CG:29:ILE:HG12  | 2.10                     | 0.51              |
| 10:CJ:7:ARG:HD3    | 10:CJ:75:ASP:OD1  | 2.11                     | 0.51              |
| 22:DA:1068:G:H2'   | 22:DA:1096:A:C5'  | 2.40                     | 0.51              |
| 22:DA:122:G:H2'    | 22:DA:123:G:O4'   | 2.10                     | 0.51              |
| 22:DA:1344:U:HO2'  | 22:DA:1345:C:P    | 2.30                     | 0.51              |
| 22:DA:1740:G:C2    | 22:DA:1741:C:C2   | 2.99                     | 0.51              |
| 22:DA:1789:A:H5''  | 24:DC:219:THR:O   | 2.10                     | 0.51              |
| 22:DA:1798:U:O2'   | 22:DA:1802:A:N3   | 2.41                     | 0.51              |
| 22:DA:1853:A:N3    | 22:DA:2233:U:O2'  | 2.36                     | 0.51              |
| 22:DA:193:U:C5     | 22:DA:194:G:N7    | 2.79                     | 0.51              |
| 22:DA:2024:G:C4    | 22:DA:2040:G:N2   | 2.79                     | 0.51              |
| 22:DA:186:G:N2     | 22:DA:211:C:C2    | 2.78                     | 0.51              |
| 22:DA:2507:C:C4    | 22:DA:2508:G:C5   | 2.99                     | 0.51              |
| 22:DA:2624:G:H1'   | 48:D0:19:HIS:HE1  | 1.75                     | 0.51              |
| 22:DA:2739:U:C5    | 22:DA:2763:G:C5   | 2.98                     | 0.51              |
| 24:DC:34:LEU:O     | 24:DC:35:GLU:CB   | 2.58                     | 0.51              |
| 27:DF:147:ASP:O    | 27:DF:148:ARG:HB2 | 2.10                     | 0.51              |
| 22:DA:2531:A:C5'   | 28:DG:157:TYR:CZ  | 2.92                     | 0.51              |
| 29:DH:121:VAL:O    | 29:DH:122:LEU:HB2 | 2.11                     | 0.51              |
| 37:DP:40:LEU:HD23  | 37:DP:41:GLN:N    | 2.25                     | 0.51              |
| 42:DU:34:VAL:O     | 42:DU:64:ALA:HA   | 2.10                     | 0.51              |
| 42:DU:67:VAL:HA    | 42:DU:70:VAL:CG2  | 2.41                     | 0.51              |
| 46:DY:48:ARG:O     | 46:DY:51:ALA:HB3  | 2.11                     | 0.51              |
| 1:AA:1238:A:C2     | 1:AA:1303:C:H4'   | 2.45                     | 0.51              |
| 1:AA:1419:G:C6     | 1:AA:1420:U:C4    | 2.98                     | 0.51              |
| 1:AA:393:A:C2      | 1:AA:394:G:C8     | 2.99                     | 0.51              |
| 1:AA:701:U:H4'     | 1:AA:702:A:C5'    | 2.40                     | 0.51              |
| 1:AA:957:U:C2      | 1:AA:959:A:OP2    | 2.63                     | 0.51              |
| 3:AC:25:ASN:O      | 3:AC:27:LYS:N     | 2.42                     | 0.51              |
| 1:AA:545:C:H5'     | 4:AD:69:GLU:CG    | 2.41                     | 0.51              |
| 20:AT:44:LYS:HG2   | 20:AT:87:ALA:CB   | 2.40                     | 0.51              |
| 21:AU:20:LYS:CE    | 21:AU:20:LYS:HA   | 2.40                     | 0.51              |
| 22:BA:1586:A:N7    | 22:BA:1587:G:C8   | 2.78                     | 0.51              |
| 22:BA:1850:G:C6    | 22:BA:1851:U:C4   | 2.98                     | 0.51              |
| 22:BA:1880:U:H2'   | 22:BA:1881:C:C6   | 2.46                     | 0.51              |
| 22:BA:1996:C:H4'   | 22:BA:1997:C:OP1  | 2.10                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:BA:2033:A:H4'  | 22:BA:2034:U:OP1  | 2.10                     | 0.51              |
| 22:BA:2140:G:N3   | 22:BA:2140:G:H2'  | 2.25                     | 0.51              |
| 22:BA:2558:C:C2'  | 22:BA:2559:C:H5'  | 2.41                     | 0.51              |
| 22:BA:2703:C:H2'  | 22:BA:2704:C:H6   | 1.75                     | 0.51              |
| 29:BH:85:GLY:HA2  | 29:BH:91:PHE:CE2  | 2.46                     | 0.51              |
| 29:BH:99:ILE:O    | 29:BH:103:VAL:CG2 | 2.58                     | 0.51              |
| 42:BU:72:ILE:HD12 | 42:BU:72:ILE:O    | 2.09                     | 0.51              |
| 1:CA:474:G:H2'    | 1:CA:475:C:O4'    | 2.11                     | 0.51              |
| 1:CA:597:G:H2'    | 1:CA:598:U:H5'    | 1.92                     | 0.51              |
| 4:CD:29:ASP:O     | 4:CD:30:THR:C     | 2.49                     | 0.51              |
| 10:CJ:52:LEU:HB2  | 14:CN:81:ARG:HD2  | 1.92                     | 0.51              |
| 12:CL:40:THR:HG22 | 12:CL:41:THR:N    | 2.26                     | 0.51              |
| 12:CL:38:TYR:HB2  | 12:CL:52:VAL:HG13 | 1.92                     | 0.51              |
| 14:CN:80:SER:O    | 14:CN:83:LYS:N    | 2.43                     | 0.51              |
| 1:CA:1014:A:O4'   | 19:CS:34:TRP:CZ3  | 2.63                     | 0.51              |
| 22:DA:1178:C:C2   | 22:DA:1179:G:N7   | 2.79                     | 0.51              |
| 22:DA:1213:A:N3   | 22:DA:1238:G:O2'  | 2.40                     | 0.51              |
| 22:DA:1330:C:O2'  | 22:DA:1331:G:H5'  | 2.10                     | 0.51              |
| 22:DA:1528:A:N6   | 22:DA:1543:G:O2'  | 2.44                     | 0.51              |
| 22:DA:2461:A:C2   | 22:DA:2490:G:N2   | 2.78                     | 0.51              |
| 22:DA:669:G:N2    | 22:DA:670:A:N1    | 2.58                     | 0.51              |
| 29:DH:26:ALA:HA   | 29:DH:30:LEU:HB2  | 1.92                     | 0.51              |
| 32:DK:28:SER:O    | 32:DK:29:HIS:HB2  | 2.09                     | 0.51              |
| 1:AA:1350:A:OP1   | 9:AI:123:ARG:NE   | 2.44                     | 0.51              |
| 1:AA:392:C:C2     | 1:AA:393:A:C8     | 2.99                     | 0.51              |
| 12:AL:44:LYS:HB3  | 12:AL:45:PRO:CD   | 2.40                     | 0.51              |
| 16:AP:51:ARG:HH11 | 16:AP:51:ARG:CG   | 2.24                     | 0.51              |
| 16:AP:70:ARG:O    | 16:AP:70:ARG:HG3  | 2.09                     | 0.51              |
| 16:AP:79:ASN:O    | 16:AP:80:LYS:HE3  | 2.10                     | 0.51              |
| 17:AQ:45:HIS:CB   | 17:AQ:70:THR:HG22 | 2.41                     | 0.51              |
| 22:BA:141:G:H5''  | 22:BA:142:A:C6    | 2.45                     | 0.51              |
| 22:BA:2177:C:O2'  | 53:B5:47:LYS:NZ   | 2.39                     | 0.51              |
| 22:BA:2266:A:H4'  | 22:BA:2267:A:O5'  | 2.11                     | 0.51              |
| 22:BA:2267:A:H2   | 57:BA:3514:HOH:O  | 1.93                     | 0.51              |
| 29:BH:117:LEU:CD2 | 29:BH:121:VAL:N   | 2.70                     | 0.51              |
| 29:BH:132:PHE:O   | 29:BH:139:PHE:HB3 | 2.11                     | 0.51              |
| 29:BH:94:ILE:CG2  | 29:BH:99:ILE:CG1  | 2.88                     | 0.51              |
| 30:BI:86:ILE:N    | 30:BI:86:ILE:HD12 | 2.26                     | 0.51              |
| 39:BR:37:GLU:OE2  | 39:BR:53:PHE:CE2  | 2.64                     | 0.51              |
| 1:CA:1067:A:N1    | 1:CA:1108:G:O2'   | 2.28                     | 0.51              |
| 1:CA:1068:G:H2'   | 1:CA:1069:C:H5'   | 1.92                     | 0.51              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:1133:G:H2'    | 1:CA:1133:G:N3     | 2.26                     | 0.51              |
| 1:CA:409:U:H2'     | 1:CA:410:G:O4'     | 2.10                     | 0.51              |
| 3:CC:62:LYS:O      | 3:CC:97:VAL:HB     | 2.10                     | 0.51              |
| 1:CA:1291:U:OP1    | 7:CG:37:SER:HB3    | 2.10                     | 0.51              |
| 12:CL:24:LEU:HD22  | 12:CL:59:ASN:OD1   | 2.11                     | 0.51              |
| 12:CL:61:PHE:CD1   | 12:CL:61:PHE:N     | 2.75                     | 0.51              |
| 20:CT:3:ASN:N      | 20:CT:8:LYS:HD3    | 2.26                     | 0.51              |
| 22:DA:125:A:H3'    | 50:D2:19:ARG:HG3   | 1.93                     | 0.51              |
| 22:DA:1519:G:C6    | 22:DA:1520:U:C2    | 2.99                     | 0.51              |
| 22:DA:1827:U:H2'   | 22:DA:1828:G:O5'   | 2.10                     | 0.51              |
| 22:DA:310:A:O2'    | 22:DA:311:A:P      | 2.67                     | 0.51              |
| 22:DA:914:G:H5'    | 22:DA:915:C:OP2    | 2.10                     | 0.51              |
| 24:DC:9:THR:O      | 24:DC:10:SER:HB3   | 2.10                     | 0.51              |
| 25:DD:114:LYS:HE2  | 25:DD:196:ALA:CB   | 2.41                     | 0.51              |
| 26:DE:108:ILE:HD13 | 26:DE:181:ILE:HG12 | 1.91                     | 0.51              |
| 29:DH:53:GLU:O     | 29:DH:54:LEU:C     | 2.49                     | 0.51              |
| 33:DL:135:ILE:O    | 33:DL:140:GLY:HA3  | 2.09                     | 0.51              |
| 37:DP:39:ARG:HG3   | 37:DP:40:LEU:N     | 2.26                     | 0.51              |
| 22:DA:85:G:OP2     | 42:DU:28:VAL:HG12  | 2.11                     | 0.51              |
| 45:DX:54:LYS:O     | 45:DX:57:ARG:N     | 2.42                     | 0.51              |
| 1:AA:1154:G:H2'    | 1:AA:1155:A:C8     | 2.46                     | 0.51              |
| 1:AA:887:G:C2'     | 1:AA:888:G:H5'     | 2.40                     | 0.51              |
| 2:AB:50:PHE:CA     | 2:AB:213:TYR:OH    | 2.58                     | 0.51              |
| 3:AC:155:GLY:N     | 3:AC:164:ARG:O     | 2.43                     | 0.51              |
| 10:AJ:15:HIS:CG    | 10:AJ:16:ARG:N     | 2.79                     | 0.51              |
| 11:AK:88:GLY:H     | 11:AK:114:THR:HG22 | 1.76                     | 0.51              |
| 16:AP:50:THR:O     | 16:AP:50:THR:CG2   | 2.57                     | 0.51              |
| 1:AA:130:A:N7      | 17:AQ:65:ARG:HB2   | 2.25                     | 0.51              |
| 53:B5:122:GLY:HA3  | 53:B5:146:VAL:CB   | 2.41                     | 0.51              |
| 22:BA:1274:A:N1    | 22:BA:1644:C:O2'   | 2.29                     | 0.51              |
| 22:BA:1415:U:O2    | 22:BA:1415:U:H2'   | 2.11                     | 0.51              |
| 22:BA:1949:G:C2    | 22:BA:1958:C:O2    | 2.64                     | 0.51              |
| 22:BA:693:A:O2'    | 22:BA:694:U:H5'    | 2.11                     | 0.51              |
| 33:BL:91:ASP:O     | 33:BL:94:THR:HB    | 2.11                     | 0.51              |
| 22:BA:2019:A:H4'   | 38:BQ:34:VAL:HG21  | 1.93                     | 0.51              |
| 1:CA:1084:G:C5     | 1:CA:1085:U:C4     | 2.98                     | 0.51              |
| 1:CA:1089:G:C4     | 1:CA:1090:U:C6     | 2.99                     | 0.51              |
| 1:CA:402:G:H4'     | 1:CA:620:C:O2      | 2.11                     | 0.51              |
| 3:CC:87:LEU:HA     | 3:CC:90:VAL:HG22   | 1.93                     | 0.51              |
| 4:CD:173:VAL:HG13  | 4:CD:174:ASP:N     | 2.26                     | 0.51              |
| 5:CE:19:ASN:O      | 5:CE:33:PHE:HA     | 2.10                     | 0.51              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 10:CJ:17:LEU:HD23  | 10:CJ:18:ILE:N    | 2.25                     | 0.51              |
| 16:CP:14:ARG:N     | 16:CP:15:PRO:HD2  | 2.25                     | 0.51              |
| 22:DA:121:G:H1'    | 22:DA:131:A:C2    | 2.45                     | 0.51              |
| 22:DA:762:U:N3     | 22:DA:1431:A:OP1  | 2.44                     | 0.51              |
| 22:DA:1737:G:O6    | 22:DA:1738:G:N1   | 2.42                     | 0.51              |
| 22:DA:531:C:C5     | 22:DA:2035:G:C2   | 2.98                     | 0.51              |
| 22:DA:207:A:H2'    | 22:DA:207:A:N3    | 2.25                     | 0.51              |
| 22:DA:2164:C:H2'   | 22:DA:2165:C:C5   | 2.45                     | 0.51              |
| 22:DA:2645:G:H3'   | 22:DA:2646:C:C5'  | 2.38                     | 0.51              |
| 22:DA:38:A:C2      | 22:DA:442:G:C6    | 2.99                     | 0.51              |
| 22:DA:37:C:H2'     | 22:DA:38:A:O4'    | 2.11                     | 0.51              |
| 22:DA:647:G:N7     | 22:DA:648:G:N7    | 2.59                     | 0.51              |
| 22:DA:681:G:C2     | 22:DA:797:G:C2    | 2.98                     | 0.51              |
| 30:DI:51:LYS:N     | 30:DI:51:LYS:HD3  | 2.25                     | 0.51              |
| 33:DL:117:THR:HG22 | 33:DL:118:THR:N   | 2.25                     | 0.51              |
| 1:AA:495:A:C2      | 1:AA:496:A:N6     | 2.79                     | 0.51              |
| 1:AA:702:A:H3'     | 1:AA:703:G:C5'    | 2.40                     | 0.51              |
| 1:AA:961:U:C4      | 1:AA:962:C:C5     | 2.98                     | 0.51              |
| 4:AD:170:TRP:O     | 4:AD:183:LYS:HB3  | 2.10                     | 0.51              |
| 5:AE:101:GLU:CB    | 5:AE:122:ASN:CB   | 2.87                     | 0.51              |
| 20:AT:58:VAL:CG1   | 20:AT:72:ALA:CB   | 2.89                     | 0.51              |
| 22:BA:752:A:H3'    | 50:B2:1:MET:SD    | 2.51                     | 0.51              |
| 22:BA:2526:G:C2'   | 52:B4:1:MET:H1    | 2.23                     | 0.51              |
| 53:B5:52:PRO:O     | 53:B5:53:ARG:CB   | 2.59                     | 0.51              |
| 22:BA:1559:U:H4'   | 22:BA:1560:G:OP2  | 2.10                     | 0.51              |
| 22:BA:2310:C:C4    | 27:BF:77:PHE:CZ   | 2.99                     | 0.51              |
| 22:BA:2326:C:H1'   | 22:BA:2327:A:OP1  | 2.11                     | 0.51              |
| 22:BA:2341:G:H2'   | 22:BA:2342:C:C6   | 2.46                     | 0.51              |
| 22:BA:71:A:H5''    | 22:BA:72:U:H3'    | 1.93                     | 0.51              |
| 22:BA:947:A:O2'    | 22:BA:984:A:C2    | 2.61                     | 0.51              |
| 29:BH:100:ALA:CB   | 29:BH:112:LYS:HA  | 2.41                     | 0.51              |
| 30:BI:62:TYR:O     | 30:BI:63:ALA:HB2  | 2.10                     | 0.51              |
| 32:BK:116:ILE:HG13 | 32:BK:117:SER:N   | 2.26                     | 0.51              |
| 36:BO:94:ARG:O     | 36:BO:96:GLY:N    | 2.43                     | 0.51              |
| 40:BS:20:VAL:HA    | 40:BS:23:LEU:HD12 | 1.92                     | 0.51              |
| 41:BT:51:PHE:O     | 41:BT:52:GLU:C    | 2.48                     | 0.51              |
| 45:BX:43:GLU:OE2   | 45:BX:45:ARG:NH2  | 2.43                     | 0.51              |
| 1:CA:1004:A:C6     | 1:CA:1005:A:C6    | 2.98                     | 0.51              |
| 2:CB:102:THR:HB    | 2:CB:175:GLU:CG   | 2.41                     | 0.51              |
| 5:CE:78:ASN:OD1    | 5:CE:79:GLY:N     | 2.44                     | 0.51              |
| 8:CH:86:TYR:CD2    | 8:CH:124:GLU:HB2  | 2.45                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:CK:35:THR:OG1  | 11:CK:40:ASN:N    | 2.44                     | 0.51              |
| 22:DA:1222:U:H1'  | 22:DA:1228:G:N2   | 2.26                     | 0.51              |
| 22:DA:1734:G:H2'  | 22:DA:1735:A:C8   | 2.46                     | 0.51              |
| 22:DA:2145:C:H5'' | 22:DA:2146:C:P    | 2.51                     | 0.51              |
| 22:DA:2324:U:O2   | 22:DA:2385:C:C5   | 2.64                     | 0.51              |
| 22:DA:2531:A:H5'  | 28:DG:157:TYR:CE2 | 2.46                     | 0.51              |
| 22:DA:2740:A:N6   | 22:DA:2764:A:C8   | 2.79                     | 0.51              |
| 22:DA:635:C:O2'   | 22:DA:639:U:H5''  | 2.10                     | 0.51              |
| 22:DA:1567:G:C8   | 24:DC:83:TYR:CD1  | 2.98                     | 0.51              |
| 22:DA:1671:U:H1'  | 25:DD:134:HIS:CE1 | 2.46                     | 0.51              |
| 27:DF:2:ALA:N     | 27:DF:94:GLU:OE2  | 2.43                     | 0.51              |
| 30:DI:54:PRO:HG2  | 30:DI:78:VAL:HB   | 1.92                     | 0.51              |
| 31:DJ:42:ALA:O    | 38:DQ:64:ARG:HD3  | 2.10                     | 0.51              |
| 38:DQ:86:ALA:O    | 38:DQ:87:SER:CB   | 2.59                     | 0.51              |
| 1:AA:1040:U:H2'   | 1:AA:1041:G:C8    | 2.46                     | 0.51              |
| 1:AA:737:C:H2'    | 1:AA:738:C:H6     | 1.75                     | 0.51              |
| 1:AA:858:G:O2'    | 1:AA:859:G:C5'    | 2.59                     | 0.51              |
| 2:AB:22:TYR:CD1   | 2:AB:22:TYR:N     | 2.78                     | 0.51              |
| 5:AE:14:LYS:CE    | 5:AE:116:GLU:OE2  | 2.59                     | 0.51              |
| 16:AP:75:ILE:HG22 | 16:AP:80:LYS:CE   | 2.40                     | 0.51              |
| 19:AS:11:ILE:HG13 | 19:AS:15:LEU:HD23 | 1.91                     | 0.51              |
| 20:AT:5:LYS:O     | 20:AT:6:SER:C     | 2.49                     | 0.51              |
| 52:B4:37:GLN:HG2  | 52:B4:37:GLN:O    | 2.10                     | 0.51              |
| 22:BA:1735:A:N3   | 22:BA:1735:A:H2'  | 2.25                     | 0.51              |
| 22:BA:2555:U:C5   | 22:BA:2556:C:N1   | 2.79                     | 0.51              |
| 22:BA:662:G:O3'   | 33:BL:16:GLY:HA2  | 2.11                     | 0.51              |
| 22:BA:869:G:H2'   | 22:BA:870:U:O4'   | 2.11                     | 0.51              |
| 29:BH:117:LEU:CD2 | 29:BH:121:VAL:CA  | 2.89                     | 0.51              |
| 22:BA:1138:G:O2'  | 31:BJ:107:GLY:HA3 | 2.11                     | 0.51              |
| 1:CA:121:U:H3'    | 1:CA:122:G:C5'    | 2.41                     | 0.51              |
| 1:CA:211:G:N3     | 1:CA:211:G:H2'    | 2.25                     | 0.51              |
| 1:CA:32:A:C2      | 1:CA:33:A:C4      | 2.98                     | 0.51              |
| 1:CA:618:C:H5''   | 1:CA:619:U:H5''   | 1.92                     | 0.51              |
| 1:CA:728:A:C8     | 15:CO:54:ARG:NH1  | 2.78                     | 0.51              |
| 1:CA:72:A:C6      | 1:CA:73:C:C4      | 2.99                     | 0.51              |
| 1:CA:840:C:C4     | 1:CA:842:U:H4'    | 2.46                     | 0.51              |
| 1:CA:861:G:C5     | 1:CA:862:C:C5     | 2.98                     | 0.51              |
| 2:CB:94:HIS:CD2   | 2:CB:146:ASN:HB2  | 2.45                     | 0.51              |
| 4:CD:11:LEU:HD23  | 4:CD:11:LEU:N     | 2.25                     | 0.51              |
| 4:CD:168:PRO:HB2  | 4:CD:171:LEU:CD1  | 2.41                     | 0.51              |
| 21:CU:53:VAL:HG13 | 21:CU:54:LYS:N    | 2.26                     | 0.51              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:DA:1109:C:C4   | 22:DA:1110:G:C6    | 2.99                     | 0.51              |
| 22:DA:1413:A:C2   | 22:DA:1590:A:C2    | 2.98                     | 0.51              |
| 22:DA:1601:G:C5   | 22:DA:1602:U:C4    | 2.99                     | 0.51              |
| 22:DA:1651:G:H4'  | 35:DN:39:PRO:HG2   | 1.93                     | 0.51              |
| 22:DA:1850:G:O6   | 22:DA:1892:C:N3    | 2.44                     | 0.51              |
| 22:DA:677:A:O2'   | 22:DA:2071:A:H5'   | 2.11                     | 0.51              |
| 26:DE:23:PHE:CG   | 26:DE:111:GLU:HG3  | 2.46                     | 0.51              |
| 29:DH:5:LEU:HA    | 29:DH:36:ALA:HA    | 1.93                     | 0.51              |
| 30:DI:28:LEU:C    | 30:DI:28:LEU:HD12  | 2.31                     | 0.51              |
| 35:DN:84:GLY:N    | 35:DN:85:PRO:CD    | 2.73                     | 0.51              |
| 1:AA:760:G:N7     | 1:AA:761:G:N7      | 2.58                     | 0.51              |
| 1:AA:575:G:C6     | 1:AA:821:G:N7      | 2.78                     | 0.51              |
| 2:AB:79:ALA:O     | 2:AB:214:LEU:CD2   | 2.59                     | 0.51              |
| 2:AB:68:LEU:HD22  | 2:AB:70:VAL:HG23   | 1.93                     | 0.51              |
| 4:AD:26:ARG:HD2   | 4:AD:31:LYS:CD     | 2.41                     | 0.51              |
| 6:AF:18:VAL:N     | 6:AF:19:PRO:HD2    | 2.26                     | 0.51              |
| 8:AH:18:GLN:O     | 8:AH:21:ASN:N      | 2.44                     | 0.51              |
| 9:AI:40:GLY:O     | 9:AI:41:ARG:CB     | 2.59                     | 0.51              |
| 9:AI:86:ALA:C     | 9:AI:88:MET:N      | 2.63                     | 0.51              |
| 19:AS:14:HIS:O    | 19:AS:18:LYS:HB2   | 2.11                     | 0.51              |
| 22:BA:1411:U:H2'  | 22:BA:1412:U:O4'   | 2.10                     | 0.51              |
| 22:BA:1824:G:N3   | 24:BC:252:THR:HG21 | 2.26                     | 0.51              |
| 22:BA:2291:U:H2'  | 22:BA:2292:U:C5    | 2.45                     | 0.51              |
| 22:BA:2507:C:H5'' | 22:BA:2573:C:N4    | 2.26                     | 0.51              |
| 22:BA:2669:G:O2'  | 22:BA:2670:A:H5'   | 2.11                     | 0.51              |
| 22:BA:404:A:H1'   | 22:BA:405:U:OP2    | 2.10                     | 0.51              |
| 22:BA:480:A:C2'   | 22:BA:481:G:OP1    | 2.59                     | 0.51              |
| 27:BF:122:PHE:HB3 | 27:BF:163:ASP:OD2  | 2.09                     | 0.51              |
| 29:BH:83:LYS:HA   | 29:BH:148:ALA:HA   | 1.93                     | 0.51              |
| 38:BQ:76:TYR:CZ   | 38:BQ:80:ILE:HG13  | 2.46                     | 0.51              |
| 1:CA:1105:A:C2    | 1:CA:1106:G:C8     | 2.99                     | 0.51              |
| 1:CA:1053:G:N7    | 1:CA:1200:C:H5'    | 2.26                     | 0.51              |
| 1:CA:913:A:H4'    | 1:CA:914:A:OP1     | 2.11                     | 0.51              |
| 2:CB:85:LEU:CG    | 2:CB:85:LEU:O      | 2.59                     | 0.51              |
| 5:CE:83:HIS:NE2   | 8:CH:96:MET:HE3    | 2.26                     | 0.51              |
| 6:CF:22:ILE:O     | 6:CF:26:THR:OG1    | 2.27                     | 0.51              |
| 22:DA:1304:A:C6   | 22:DA:1305:C:C4    | 2.99                     | 0.51              |
| 22:DA:1876:A:C8   | 22:DA:1877:A:N7    | 2.79                     | 0.51              |
| 22:DA:2621:G:OP1  | 25:DD:124:ARG:NH2  | 2.44                     | 0.51              |
| 22:DA:2843:G:N2   | 22:DA:2875:C:N3    | 2.59                     | 0.51              |
| 22:DA:532:A:N3    | 22:DA:532:A:H2'    | 2.26                     | 0.51              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 27:DF:44:ILE:CG2  | 27:DF:79:ILE:HG22  | 2.41                     | 0.51              |
| 32:DK:47:ILE:HB   | 32:DK:48:PRO:HD2   | 1.92                     | 0.51              |
| 35:DN:51:LEU:N    | 35:DN:51:LEU:HD23  | 2.25                     | 0.51              |
| 36:DO:7:ARG:CD    | 36:DO:97:PHE:CE1   | 2.93                     | 0.51              |
| 22:DA:17:G:H4'    | 38:DQ:25:TYR:CE1   | 2.46                     | 0.51              |
| 38:DQ:61:TRP:HB3  | 38:DQ:92:ARG:O     | 2.11                     | 0.51              |
| 1:AA:1093:A:OP2   | 7:AG:4:ARG:NH2     | 2.44                     | 0.51              |
| 1:AA:71:A:H3'     | 1:AA:71:A:OP2      | 2.10                     | 0.51              |
| 1:AA:862:C:C2'    | 1:AA:863:U:H5'     | 2.40                     | 0.51              |
| 1:AA:903:G:H2'    | 1:AA:904:U:C6      | 2.45                     | 0.51              |
| 1:AA:949:A:C5     | 1:AA:950:U:C5      | 2.99                     | 0.51              |
| 2:AB:64:LYS:HD3   | 2:AB:64:LYS:C      | 2.31                     | 0.51              |
| 3:AC:11:ARG:O     | 3:AC:12:LEU:C      | 2.48                     | 0.51              |
| 7:AG:99:LEU:O     | 7:AG:100:ALA:C     | 2.49                     | 0.51              |
| 8:AH:89:LYS:HG3   | 8:AH:90:ASP:N      | 2.26                     | 0.51              |
| 14:AN:31:ILE:CG2  | 14:AN:31:ILE:O     | 2.58                     | 0.51              |
| 14:AN:61:ARG:O    | 14:AN:62:ASN:CB    | 2.58                     | 0.51              |
| 22:BA:1088:A:H5'' | 22:BA:1088:A:N3    | 2.25                     | 0.51              |
| 22:BA:1495:A:C6   | 22:BA:1496:A:C6    | 2.99                     | 0.51              |
| 22:BA:1651:G:O6   | 57:BA:3798:HOH:O   | 2.20                     | 0.51              |
| 24:BC:195:VAL:CG1 | 24:BC:196:GLY:N    | 2.73                     | 0.51              |
| 22:BA:636:G:C6    | 33:BL:111:ILE:HD11 | 2.45                     | 0.51              |
| 36:BO:88:LYS:HA   | 36:BO:115:LEU:HD12 | 1.93                     | 0.51              |
| 36:BO:2:ASP:OD1   | 36:BO:3:LYS:N      | 2.44                     | 0.51              |
| 38:BQ:88:VAL:HG13 | 39:BR:49:ILE:HD11  | 1.93                     | 0.51              |
| 43:BV:72:VAL:HG12 | 43:BV:93:ARG:HA    | 1.93                     | 0.51              |
| 1:CA:1463:U:H2'   | 1:CA:1464:U:C6     | 2.46                     | 0.51              |
| 1:CA:1505:G:H4'   | 1:CA:1506:U:H5''   | 1.93                     | 0.51              |
| 1:CA:115:G:C2     | 1:CA:289:G:N7      | 2.78                     | 0.51              |
| 1:CA:4:U:H2'      | 1:CA:4:U:O2        | 2.10                     | 0.51              |
| 1:CA:747:A:N6     | 1:CA:748:G:C6      | 2.79                     | 0.51              |
| 1:CA:756:C:O2'    | 1:CA:757:U:H5'     | 2.11                     | 0.51              |
| 11:CK:31:ILE:HB   | 11:CK:46:THR:HG22  | 1.93                     | 0.51              |
| 16:CP:75:ILE:HA   | 16:CP:78:VAL:HG12  | 1.92                     | 0.51              |
| 1:CA:332:G:OP2    | 20:CT:5:LYS:HB3    | 2.11                     | 0.51              |
| 21:CU:44:GLU:OE1  | 21:CU:45:ARG:NH1   | 2.44                     | 0.51              |
| 22:DA:1257:C:N4   | 22:DA:1258:U:O4    | 2.43                     | 0.51              |
| 22:DA:1343:G:C5   | 22:DA:1344:U:O4    | 2.64                     | 0.51              |
| 22:DA:1351:C:H2'  | 22:DA:1352:U:C1'   | 2.41                     | 0.51              |
| 22:DA:1866:A:N3   | 22:DA:1876:A:C6    | 2.79                     | 0.51              |
| 22:DA:2186:G:C5   | 22:DA:2187:U:C5    | 2.99                     | 0.51              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:DA:2326:C:C1'  | 22:DA:2327:A:OP1  | 2.59                     | 0.51              |
| 22:DA:559:G:N3    | 38:DQ:56:GLN:NE2  | 2.59                     | 0.51              |
| 22:DA:622:G:H2'   | 22:DA:623:C:C6    | 2.46                     | 0.51              |
| 22:DA:675:A:H4'   | 26:DE:62:GLN:OE1  | 2.11                     | 0.51              |
| 22:DA:836:G:C5    | 22:DA:837:C:C4    | 2.99                     | 0.51              |
| 32:DK:41:ILE:HD11 | 32:DK:86:LEU:CD2  | 2.40                     | 0.51              |
| 43:DV:80:HIS:CE1  | 43:DV:83:LYS:HB2  | 2.46                     | 0.51              |
| 1:AA:1535:C:C6    | 1:AA:1535:C:OP2   | 2.64                     | 0.50              |
| 1:AA:947:G:C5     | 1:AA:948:C:C4     | 2.99                     | 0.50              |
| 10:AJ:30:LYS:HA   | 10:AJ:34:ALA:HA   | 1.92                     | 0.50              |
| 22:BA:1073:A:OP1  | 22:BA:1073:A:C8   | 2.64                     | 0.50              |
| 22:BA:1098:A:N7   | 22:BA:1099:G:O6   | 2.44                     | 0.50              |
| 22:BA:1439:A:C8   | 22:BA:1440:U:C6   | 2.98                     | 0.50              |
| 22:BA:1606:C:HO2' | 22:BA:1607:C:P    | 2.34                     | 0.50              |
| 22:BA:1870:C:H4'  | 22:BA:1871:A:OP2  | 2.10                     | 0.50              |
| 22:BA:1924:C:OP2  | 22:BA:1924:C:H3'  | 2.11                     | 0.50              |
| 22:BA:2086:U:H2'  | 22:BA:2087:G:C8   | 2.46                     | 0.50              |
| 22:BA:543:G:C2    | 22:BA:544:C:H1'   | 2.47                     | 0.50              |
| 23:BB:35:C:H2'    | 23:BB:36:C:H5'    | 1.93                     | 0.50              |
| 23:BB:78:A:H2'    | 23:BB:79:G:O4'    | 2.10                     | 0.50              |
| 24:BC:72:ASP:HA   | 24:BC:118:SER:O   | 2.11                     | 0.50              |
| 25:BD:36:GLN:OE1  | 25:BD:67:HIS:HE1  | 1.94                     | 0.50              |
| 30:BI:116:ASP:O   | 30:BI:117:MET:HB2 | 2.11                     | 0.50              |
| 46:BY:42:LEU:O    | 46:BY:45:GLN:O    | 2.29                     | 0.50              |
| 2:CB:135:LEU:O    | 2:CB:139:ARG:HG3  | 2.11                     | 0.50              |
| 4:CD:148:LYS:CD   | 4:CD:148:LYS:H    | 2.24                     | 0.50              |
| 7:CG:46:ALA:HB2   | 7:CG:117:ALA:HA   | 1.92                     | 0.50              |
| 8:CH:20:ALA:O     | 8:CH:22:LYS:N     | 2.44                     | 0.50              |
| 1:CA:653:U:C2     | 8:CH:56:LYS:HG2   | 2.46                     | 0.50              |
| 17:CQ:61:ILE:HG23 | 17:CQ:73:TRP:CE3  | 2.45                     | 0.50              |
| 22:DA:250:G:OP2   | 51:D3:13:ARG:NH1  | 2.44                     | 0.50              |
| 22:DA:1076:C:H2'  | 22:DA:1077:A:O4'  | 2.12                     | 0.50              |
| 22:DA:1317:G:C6   | 22:DA:1318:U:N3   | 2.79                     | 0.50              |
| 22:DA:142:A:C5    | 22:DA:143:C:N4    | 2.79                     | 0.50              |
| 22:DA:1616:A:H2   | 22:DA:1647:U:C5   | 2.28                     | 0.50              |
| 22:DA:1607:C:O2   | 22:DA:1621:U:C5   | 2.64                     | 0.50              |
| 22:DA:410:G:H2'   | 22:DA:2407:A:C8   | 2.46                     | 0.50              |
| 22:DA:658:U:N3    | 22:DA:659:G:N7    | 2.59                     | 0.50              |
| 30:DI:6:GLN:O     | 30:DI:7:ALA:HB3   | 2.10                     | 0.50              |
| 37:DP:51:ARG:HG3  | 37:DP:51:ARG:O    | 2.11                     | 0.50              |
| 44:DW:36:ILE:HG23 | 44:DW:58:THR:CG2  | 2.40                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 44:DW:45:PHE:CD2  | 44:DW:80:ILE:CD1  | 2.94                     | 0.50              |
| 1:AA:1037:C:H2'   | 1:AA:1038:C:C6    | 2.46                     | 0.50              |
| 1:AA:1397:C:O2'   | 1:AA:1398:A:OP1   | 2.27                     | 0.50              |
| 1:AA:1450:U:H2'   | 1:AA:1452:C:C5    | 2.46                     | 0.50              |
| 1:AA:764:C:H2'    | 1:AA:765:G:O4'    | 2.12                     | 0.50              |
| 2:AB:21:ARG:NE    | 2:AB:21:ARG:HA    | 2.26                     | 0.50              |
| 2:AB:59:LYS:O     | 2:AB:63:ARG:HG3   | 2.12                     | 0.50              |
| 16:AP:10:GLY:O    | 16:AP:11:ALA:HB2  | 2.11                     | 0.50              |
| 21:AU:18:ARG:HD2  | 21:AU:18:ARG:N    | 2.26                     | 0.50              |
| 21:AU:35:ARG:O    | 21:AU:36:GLU:C    | 2.48                     | 0.50              |
| 53:B5:68:GLY:O    | 53:B5:70:GLY:N    | 2.44                     | 0.50              |
| 22:BA:1586:A:C8   | 22:BA:1587:G:C8   | 2.98                     | 0.50              |
| 22:BA:1845:G:C6   | 22:BA:1896:G:C6   | 2.99                     | 0.50              |
| 22:BA:1916:A:OP2  | 22:BA:1916:A:H3'  | 2.11                     | 0.50              |
| 22:BA:1917:U:H2'  | 22:BA:1917:U:O2   | 2.10                     | 0.50              |
| 22:BA:2217:G:O2'  | 22:BA:2218:G:H5'  | 2.11                     | 0.50              |
| 34:BM:28:PHE:HB2  | 34:BM:104:GLU:OE2 | 2.11                     | 0.50              |
| 37:BP:114:LEU:O   | 37:BP:115:ASN:HB3 | 2.11                     | 0.50              |
| 39:BR:49:ILE:O    | 39:BR:51:VAL:O    | 2.30                     | 0.50              |
| 1:CA:1010:U:C2    | 1:CA:1020:G:C2    | 3.00                     | 0.50              |
| 1:CA:518:C:H2'    | 1:CA:530:G:C8     | 2.46                     | 0.50              |
| 1:CA:667:G:C2     | 1:CA:740:U:O2     | 2.64                     | 0.50              |
| 2:CB:26:LYS:HB2   | 2:CB:193:PRO:HD2  | 1.94                     | 0.50              |
| 2:CB:56:GLU:HG2   | 2:CB:198:PHE:CZ   | 2.47                     | 0.50              |
| 7:CG:51:ALA:CB    | 7:CG:58:GLU:HA    | 2.41                     | 0.50              |
| 13:CM:4:ILE:HA    | 13:CM:57:ARG:CZ   | 2.41                     | 0.50              |
| 17:CQ:45:HIS:O    | 17:CQ:71:LYS:HA   | 2.11                     | 0.50              |
| 22:DA:1314:C:OP1  | 22:DA:1332:G:OP1  | 2.29                     | 0.50              |
| 22:DA:158:U:H2'   | 22:DA:159:G:H5'   | 1.93                     | 0.50              |
| 22:DA:1596:A:N6   | 22:DA:1597:A:C6   | 2.80                     | 0.50              |
| 22:DA:1605:C:H4'  | 22:DA:1610:A:C6   | 2.46                     | 0.50              |
| 22:DA:1736:U:H2'  | 22:DA:1737:G:O4'  | 2.11                     | 0.50              |
| 22:DA:1788:C:H2'  | 22:DA:1789:A:O4'  | 2.11                     | 0.50              |
| 22:DA:2297:A:N1   | 22:DA:2321:U:H5   | 2.09                     | 0.50              |
| 22:DA:2824:C:C4   | 22:DA:2825:G:C5   | 3.00                     | 0.50              |
| 22:DA:590:A:C5    | 22:DA:591:U:C5    | 2.99                     | 0.50              |
| 22:DA:66:C:C4     | 22:DA:67:U:C5     | 2.99                     | 0.50              |
| 22:DA:933:A:C5'   | 22:DA:934:U:OP2   | 2.59                     | 0.50              |
| 24:DC:51:THR:CG2  | 24:DC:54:ILE:HD11 | 2.41                     | 0.50              |
| 30:DI:80:LEU:HD23 | 30:DI:84:ALA:CB   | 2.41                     | 0.50              |
| 35:DN:106:ASP:O   | 35:DN:107:ASN:C   | 2.49                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 41:DT:69:ARG:HB2  | 41:DT:74:ILE:HG22 | 1.92                     | 0.50              |
| 45:DX:52:SER:OG   | 45:DX:55:GLY:N    | 2.40                     | 0.50              |
| 1:AA:1069:C:H4'   | 1:AA:1192:C:O2    | 2.11                     | 0.50              |
| 1:AA:118:U:O4     | 1:AA:288:A:H2'    | 2.12                     | 0.50              |
| 1:AA:1236:A:H4'   | 1:AA:1304:G:H4'   | 1.92                     | 0.50              |
| 1:AA:405:U:OP1    | 1:AA:406:G:O2'    | 2.21                     | 0.50              |
| 12:AL:22:PRO:C    | 12:AL:24:LEU:H    | 2.14                     | 0.50              |
| 12:AL:56:ARG:CZ   | 12:AL:62:GLU:HG3  | 2.41                     | 0.50              |
| 12:AL:88:LYS:HG3  | 12:AL:88:LYS:O    | 2.11                     | 0.50              |
| 1:AA:625:U:H5''   | 16:AP:16:PHE:CD1  | 2.47                     | 0.50              |
| 17:AQ:52:GLU:N    | 17:AQ:52:GLU:CD   | 2.64                     | 0.50              |
| 49:B1:17:THR:HG21 | 49:B1:43:VAL:HG13 | 1.94                     | 0.50              |
| 22:BA:1613:G:O2'  | 50:B2:3:ARG:HD3   | 2.11                     | 0.50              |
| 53:B5:40:GLU:O    | 53:B5:42:VAL:N    | 2.42                     | 0.50              |
| 53:B5:50:ILE:HG22 | 53:B5:51:ASP:N    | 2.26                     | 0.50              |
| 22:BA:1056:G:H5'' | 22:BA:1057:A:O4'  | 2.11                     | 0.50              |
| 22:BA:1068:G:H2'  | 22:BA:1069:A:H5'  | 1.94                     | 0.50              |
| 22:BA:2196:C:O2'  | 22:BA:2197:U:H5'  | 2.10                     | 0.50              |
| 22:BA:2243:U:P    | 57:BA:3740:HOH:O  | 2.70                     | 0.50              |
| 22:BA:2649:C:H2'  | 22:BA:2650:U:C6   | 2.45                     | 0.50              |
| 22:BA:492:A:H2'   | 22:BA:493:G:O4'   | 2.10                     | 0.50              |
| 26:BE:145:ASP:CB  | 26:BE:184:ASP:OD2 | 2.60                     | 0.50              |
| 27:BF:14:LYS:O    | 27:BF:18:THR:HG23 | 2.12                     | 0.50              |
| 32:BK:118:LEU:O   | 32:BK:119:ALA:HB3 | 2.11                     | 0.50              |
| 32:BK:4:GLU:O     | 32:BK:5:GLN:CB    | 2.57                     | 0.50              |
| 35:BN:24:MET:HE3  | 35:BN:44:LEU:HD22 | 1.94                     | 0.50              |
| 42:BU:99:ASN:OD1  | 42:BU:99:ASN:C    | 2.50                     | 0.50              |
| 1:CA:134:G:H2'    | 1:CA:135:C:O4'    | 2.11                     | 0.50              |
| 1:CA:412:A:HO2'   | 1:CA:413:G:P      | 2.33                     | 0.50              |
| 1:CA:580:C:H2'    | 1:CA:581:G:O4'    | 2.12                     | 0.50              |
| 4:CD:46:PRO:O     | 4:CD:47:ARG:C     | 2.49                     | 0.50              |
| 7:CG:88:PRO:HD2   | 7:CG:152:ALA:HA   | 1.92                     | 0.50              |
| 11:CK:72:ASP:OD1  | 11:CK:73:ALA:N    | 2.44                     | 0.50              |
| 18:CR:58:ALA:O    | 18:CR:61:ARG:N    | 2.45                     | 0.50              |
| 49:D1:21:TYR:CE1  | 49:D1:38:LYS:HD2  | 2.46                     | 0.50              |
| 22:DA:1363:C:H2'  | 22:DA:1364:G:C8   | 2.46                     | 0.50              |
| 22:DA:1453:A:C2   | 35:DN:77:ALA:CB   | 2.95                     | 0.50              |
| 22:DA:1754:A:N6   | 22:DA:1755:A:C6   | 2.79                     | 0.50              |
| 22:DA:2091:C:H1'  | 45:DX:34:HIS:CD2  | 2.46                     | 0.50              |
| 22:DA:2733:A:C2   | 22:DA:2734:A:C4   | 2.98                     | 0.50              |
| 22:DA:833:A:H2'   | 22:DA:834:G:C8    | 2.46                     | 0.50              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 29:DH:32:PRO:HB3  | 45:DX:39:TRP:HB3   | 1.93                     | 0.50              |
| 30:DI:53:LEU:HG   | 30:DI:82:LYS:HE2   | 1.92                     | 0.50              |
| 30:DI:57:VAL:CG2  | 30:DI:69:PHE:HB2   | 2.42                     | 0.50              |
| 32:DK:6:THR:O     | 32:DK:8:LEU:HD12   | 2.11                     | 0.50              |
| 39:DR:14:VAL:CG2  | 39:DR:98:ILE:HG13  | 2.42                     | 0.50              |
| 5:AE:15:LEU:HB3   | 5:AE:37:THR:CG2    | 2.42                     | 0.50              |
| 6:AF:91:ARG:CG    | 6:AF:92:THR:N      | 2.75                     | 0.50              |
| 11:AK:128:ARG:CG  | 11:AK:128:ARG:HH11 | 2.24                     | 0.50              |
| 11:AK:89:PRO:HG3  | 21:AU:29:LEU:HD21  | 1.93                     | 0.50              |
| 18:AR:63:ARG:HB3  | 18:AR:70:TYR:CZ    | 2.46                     | 0.50              |
| 20:AT:25:ARG:O    | 20:AT:29:ARG:HG2   | 2.11                     | 0.50              |
| 22:BA:1356:G:C6   | 22:BA:1357:C:C4    | 3.00                     | 0.50              |
| 22:BA:2131:U:OP2  | 22:BA:2132:U:C6    | 2.64                     | 0.50              |
| 22:BA:2449:U:H4'  | 22:BA:2450:A:OP1   | 2.11                     | 0.50              |
| 24:BC:107:PRO:HB3 | 24:BC:142:HIS:CE1  | 2.47                     | 0.50              |
| 24:BC:71:LYS:HB3  | 24:BC:96:TYR:CE2   | 2.46                     | 0.50              |
| 22:BA:321:U:C1'   | 26:BE:159:LEU:HD12 | 2.41                     | 0.50              |
| 29:BH:66:ASN:OD1  | 29:BH:138:VAL:HG21 | 2.11                     | 0.50              |
| 29:BH:80:ILE:O    | 29:BH:147:VAL:N    | 2.44                     | 0.50              |
| 30:BI:117:MET:SD  | 30:BI:129:ILE:HD11 | 2.51                     | 0.50              |
| 36:BO:36:TYR:CD2  | 36:BO:36:TYR:N     | 2.79                     | 0.50              |
| 1:CA:1007:U:H2'   | 1:CA:1008:U:H5''   | 1.92                     | 0.50              |
| 1:CA:1072:G:C5    | 1:CA:1073:U:C4     | 3.00                     | 0.50              |
| 1:CA:1096:C:H2'   | 1:CA:1097:C:H6     | 1.76                     | 0.50              |
| 1:CA:1098:C:H2'   | 1:CA:1099:G:O4'    | 2.12                     | 0.50              |
| 1:CA:1167:A:C8    | 1:CA:1169:A:C5     | 2.98                     | 0.50              |
| 1:CA:218:U:H2'    | 1:CA:219:U:O4'     | 2.12                     | 0.50              |
| 1:CA:369:G:OP2    | 1:CA:388:G:N2      | 2.43                     | 0.50              |
| 1:CA:945:G:N3     | 1:CA:945:G:H2'     | 2.25                     | 0.50              |
| 2:CB:139:ARG:HD2  | 2:CB:139:ARG:C     | 2.32                     | 0.50              |
| 3:CC:145:GLY:O    | 3:CC:146:ALA:O     | 2.29                     | 0.50              |
| 11:CK:51:GLY:O    | 11:CK:52:PHE:O     | 2.28                     | 0.50              |
| 17:CQ:25:ILE:O    | 17:CQ:41:THR:HA    | 2.11                     | 0.50              |
| 22:DA:1203:U:OP2  | 22:DA:1204:A:H2'   | 2.11                     | 0.50              |
| 22:DA:1529:G:O6   | 22:DA:1543:G:N2    | 2.44                     | 0.50              |
| 22:DA:1439:A:N7   | 22:DA:1552:A:C2    | 2.79                     | 0.50              |
| 22:DA:1791:A:H2'  | 22:DA:1792:G:H5'   | 1.94                     | 0.50              |
| 22:DA:1881:C:H2'  | 22:DA:1882:U:O4'   | 2.11                     | 0.50              |
| 22:DA:1838:C:C5   | 22:DA:1899:A:C5    | 3.00                     | 0.50              |
| 22:DA:2013:A:N6   | 22:DA:2014:A:C6    | 2.79                     | 0.50              |
| 22:DA:204:A:O4'   | 22:DA:206:U:C6     | 2.64                     | 0.50              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 22:DA:2195:U:O2'   | 22:DA:2196:C:H5'  | 2.12                     | 0.50              |
| 22:DA:498:G:C4     | 22:DA:499:U:C5    | 2.99                     | 0.50              |
| 26:DE:27:LEU:HG    | 26:DE:104:ALA:HB2 | 1.94                     | 0.50              |
| 29:DH:44:ILE:O     | 29:DH:48:GLU:HB2  | 2.12                     | 0.50              |
| 29:DH:5:LEU:HD11   | 29:DH:13:GLY:HA2  | 1.93                     | 0.50              |
| 35:DN:38:LEU:HB3   | 35:DN:39:PRO:HD3  | 1.92                     | 0.50              |
| 1:AA:1338:G:H2'    | 1:AA:1339:A:C8    | 2.47                     | 0.50              |
| 1:AA:197:A:N3      | 1:AA:198:G:H1'    | 2.26                     | 0.50              |
| 1:AA:662:U:H2'     | 1:AA:663:A:C8     | 2.46                     | 0.50              |
| 1:AA:737:C:H2'     | 1:AA:738:C:C6     | 2.46                     | 0.50              |
| 2:AB:119:THR:O     | 2:AB:120:GLN:CB   | 2.58                     | 0.50              |
| 2:AB:154:MET:O     | 2:AB:155:GLY:C    | 2.49                     | 0.50              |
| 7:AG:71:PRO:HD2    | 7:AG:96:ARG:O     | 2.12                     | 0.50              |
| 53:B5:83:LYS:HB3   | 53:B5:87:ALA:CB   | 2.41                     | 0.50              |
| 22:BA:1091:G:H2'   | 22:BA:1092:C:C5   | 2.45                     | 0.50              |
| 22:BA:136:G:C2     | 22:BA:144:A:C6    | 2.99                     | 0.50              |
| 22:BA:585:G:H5''   | 22:BA:586:A:P     | 2.52                     | 0.50              |
| 22:BA:876:C:H2'    | 22:BA:877:A:O4'   | 2.10                     | 0.50              |
| 24:BC:182:ARG:NH2  | 24:BC:266:PHE:HB3 | 2.26                     | 0.50              |
| 26:BE:149:ILE:HD12 | 26:BE:150:THR:O   | 2.10                     | 0.50              |
| 27:BF:52:ASN:HB3   | 27:BF:147:ASP:OD1 | 2.11                     | 0.50              |
| 27:BF:41:GLY:HA2   | 27:BF:85:ILE:HG13 | 1.94                     | 0.50              |
| 31:BJ:84:ILE:HG23  | 31:BJ:84:ILE:O    | 2.11                     | 0.50              |
| 33:BL:63:LYS:HA    | 51:B3:13:ARG:HG3  | 1.93                     | 0.50              |
| 38:BQ:76:TYR:CD2   | 38:BQ:76:TYR:C    | 2.85                     | 0.50              |
| 42:BU:18:ASP:O     | 42:BU:20:GLY:N    | 2.45                     | 0.50              |
| 43:BV:61:LEU:HD13  | 43:BV:61:LEU:N    | 2.26                     | 0.50              |
| 1:CA:1068:G:C6     | 1:CA:1069:C:C4    | 3.00                     | 0.50              |
| 1:CA:546:A:P       | 4:CD:69:GLU:HB3   | 2.51                     | 0.50              |
| 1:CA:81:A:C2       | 1:CA:89:U:C2      | 2.99                     | 0.50              |
| 3:CC:69:HIS:HA     | 3:CC:104:ALA:HB3  | 1.93                     | 0.50              |
| 12:CL:38:TYR:N     | 12:CL:52:VAL:O    | 2.44                     | 0.50              |
| 1:CA:846:G:OP2     | 18:CR:48:ARG:NH2  | 2.44                     | 0.50              |
| 20:CT:43:ASP:HB3   | 20:CT:46:ALA:HB3  | 1.92                     | 0.50              |
| 22:DA:1176:U:H2'   | 22:DA:1177:G:C8   | 2.47                     | 0.50              |
| 22:DA:1196:C:H1'   | 22:DA:1226:A:C4   | 2.47                     | 0.50              |
| 22:DA:1262:A:N1    | 22:DA:1263:U:C2   | 2.79                     | 0.50              |
| 22:DA:1364:G:C4    | 22:DA:1368:G:C2   | 2.99                     | 0.50              |
| 22:DA:1806:C:O2    | 24:DC:44:ASN:ND2  | 2.44                     | 0.50              |
| 22:DA:1831:G:C6    | 22:DA:1832:C:C4   | 3.00                     | 0.50              |
| 22:DA:2201:G:C6    | 22:DA:2202:U:C4   | 3.00                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:DA:2513:A:C5   | 22:DA:2514:U:C4   | 2.99                     | 0.50              |
| 22:DA:2718:G:C2   | 22:DA:2719:G:H1'  | 2.47                     | 0.50              |
| 22:DA:2720:U:C5   | 22:DA:2872:A:N1   | 2.79                     | 0.50              |
| 22:DA:329:G:O4'   | 22:DA:477:A:H1'   | 2.12                     | 0.50              |
| 22:DA:404:A:H1'   | 22:DA:405:U:OP2   | 2.12                     | 0.50              |
| 30:DI:28:LEU:HD13 | 30:DI:38:PHE:CD2  | 2.46                     | 0.50              |
| 36:DO:33:ARG:O    | 36:DO:34:HIS:CG   | 2.64                     | 0.50              |
| 1:AA:1161:C:H2'   | 1:AA:1162:C:H6    | 1.76                     | 0.50              |
| 1:AA:130:A:C8     | 17:AQ:65:ARG:HB2  | 2.46                     | 0.50              |
| 1:AA:642:A:C5     | 8:AH:107:SER:HA   | 2.47                     | 0.50              |
| 1:AA:90:C:O2'     | 1:AA:91:U:P       | 2.70                     | 0.50              |
| 2:AB:140:GLU:O    | 2:AB:144:LEU:HG   | 2.11                     | 0.50              |
| 14:AN:10:GLU:OE2  | 14:AN:61:ARG:HB3  | 2.11                     | 0.50              |
| 22:BA:1071:G:O2'  | 22:BA:1072:C:O4'  | 2.30                     | 0.50              |
| 22:BA:1168:G:C2   | 22:BA:1182:G:C4   | 2.99                     | 0.50              |
| 22:BA:1389:G:H2'  | 22:BA:1390:U:O4'  | 2.12                     | 0.50              |
| 22:BA:1794:A:C2'  | 22:BA:1795:C:O5'  | 2.59                     | 0.50              |
| 22:BA:1883:U:O4   | 22:BA:1884:G:C6   | 2.65                     | 0.50              |
| 22:BA:1786:A:C4   | 22:BA:1938:A:C6   | 3.00                     | 0.50              |
| 22:BA:1963:U:H6   | 22:BA:1963:U:O5'  | 1.95                     | 0.50              |
| 22:BA:2075:U:C4   | 22:BA:2238:G:C6   | 2.99                     | 0.50              |
| 22:BA:2512:C:H2'  | 22:BA:2513:A:O4'  | 2.11                     | 0.50              |
| 22:BA:276:U:O2    | 22:BA:276:U:H2'   | 2.11                     | 0.50              |
| 22:BA:2812:G:H2'  | 22:BA:2813:A:O4'  | 2.11                     | 0.50              |
| 22:BA:586:A:N1    | 22:BA:809:G:O2'   | 2.35                     | 0.50              |
| 22:BA:675:A:OP1   | 26:BE:58:LYS:CE   | 2.60                     | 0.50              |
| 27:BF:158:THR:CG2 | 27:BF:160:ALA:H   | 2.25                     | 0.50              |
| 36:BO:79:ALA:HB2  | 36:BO:110:ALA:HA  | 1.93                     | 0.50              |
| 38:BQ:21:ALA:HA   | 38:BQ:24:TYR:CE1  | 2.46                     | 0.50              |
| 1:CA:1474:U:H2'   | 1:CA:1475:G:H5''  | 1.93                     | 0.50              |
| 1:CA:1490:U:C2'   | 1:CA:1491:G:O4'   | 2.60                     | 0.50              |
| 1:CA:247:G:C6     | 1:CA:278:G:N1     | 2.78                     | 0.50              |
| 1:CA:298:A:H2'    | 1:CA:299:G:O4'    | 2.11                     | 0.50              |
| 12:CL:65:SER:OG   | 12:CL:97:THR:HG23 | 2.12                     | 0.50              |
| 15:CO:42:HIS:O    | 15:CO:45:GLU:O    | 2.30                     | 0.50              |
| 13:CM:79:ARG:HD2  | 19:CS:65:GLU:HG2  | 1.93                     | 0.50              |
| 22:DA:2083:G:N7   | 22:DA:2084:C:C5   | 2.80                     | 0.50              |
| 22:DA:2122:U:H2'  | 22:DA:2123:G:O4'  | 2.12                     | 0.50              |
| 22:DA:219:A:N6    | 22:DA:220:G:C6    | 2.80                     | 0.50              |
| 22:DA:24:G:C5     | 22:DA:25:U:C5     | 2.99                     | 0.50              |
| 22:DA:301:G:N3    | 22:DA:302:C:C2    | 2.80                     | 0.50              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:DA:547:A:H3'   | 22:DA:548:G:H5'    | 1.94                     | 0.50              |
| 22:DA:54:G:N1     | 22:DA:55:G:N7      | 2.60                     | 0.50              |
| 22:DA:629:G:O6    | 22:DA:630:G:C6     | 2.65                     | 0.50              |
| 26:DE:75:SER:O    | 26:DE:78:TRP:HB2   | 2.12                     | 0.50              |
| 27:DF:128:TYR:CG  | 27:DF:170:LEU:CD1  | 2.95                     | 0.50              |
| 32:DK:71:ARG:HB3  | 32:DK:72:PRO:HD2   | 1.93                     | 0.50              |
| 22:DA:2250:G:C2   | 34:DM:82:MET:HB2   | 2.47                     | 0.50              |
| 37:DP:89:ARG:O    | 37:DP:112:GLU:HA   | 2.12                     | 0.50              |
| 37:DP:75:GLN:O    | 37:DP:78:SER:HB3   | 2.11                     | 0.50              |
| 1:AA:1123:U:H4'   | 10:AJ:39:PRO:HD2   | 1.93                     | 0.50              |
| 1:AA:149:A:C2     | 1:AA:150:U:C2      | 2.99                     | 0.50              |
| 1:AA:484:G:C5     | 1:AA:486:U:H1'     | 2.47                     | 0.50              |
| 1:AA:596:A:N6     | 1:AA:645:G:C6      | 2.80                     | 0.50              |
| 1:AA:738:C:H2'    | 1:AA:739:C:H6      | 1.77                     | 0.50              |
| 2:AB:151:ILE:O    | 2:AB:152:LYS:C     | 2.50                     | 0.50              |
| 7:AG:42:ILE:HG21  | 7:AG:116:MET:CG    | 2.42                     | 0.50              |
| 13:AM:11:ASP:OD1  | 13:AM:45:ILE:HB    | 2.11                     | 0.50              |
| 22:BA:1070:A:H2'  | 22:BA:1097:U:OP1   | 2.12                     | 0.50              |
| 22:BA:1714:U:H2'  | 22:BA:1714:U:O2    | 2.11                     | 0.50              |
| 22:BA:2018:G:O2'  | 22:BA:2019:A:H5'   | 2.11                     | 0.50              |
| 22:BA:2273:A:H2'  | 22:BA:2274:A:C8    | 2.46                     | 0.50              |
| 22:BA:2297:A:N1   | 22:BA:2321:U:H5    | 2.07                     | 0.50              |
| 22:BA:769:U:C2    | 22:BA:770:G:C8     | 3.00                     | 0.50              |
| 22:BA:1800:C:H3'  | 24:BC:146:MET:HE1  | 1.94                     | 0.50              |
| 30:BI:101:ILE:O   | 30:BI:102:SER:HB2  | 2.11                     | 0.50              |
| 31:BJ:114:LEU:O   | 31:BJ:114:LEU:HD12 | 2.12                     | 0.50              |
| 31:BJ:30:THR:HG22 | 31:BJ:31:GLU:N     | 2.26                     | 0.50              |
| 36:BO:117:PHE:CD1 | 36:BO:117:PHE:O    | 2.65                     | 0.50              |
| 1:CA:206:C:C2'    | 1:CA:207:C:H5'     | 2.40                     | 0.50              |
| 1:CA:786:G:H2'    | 1:CA:786:G:N3      | 2.26                     | 0.50              |
| 1:CA:821:G:H2'    | 1:CA:822:U:H6      | 1.76                     | 0.50              |
| 3:CC:40:ARG:HG2   | 3:CC:55:ILE:HD11   | 1.94                     | 0.50              |
| 9:CI:12:ARG:CD    | 9:CI:107:ASP:HB3   | 2.42                     | 0.50              |
| 10:CJ:22:THR:HA   | 10:CJ:25:ILE:HG22  | 1.93                     | 0.50              |
| 11:CK:23:ILE:HG21 | 11:CK:96:THR:HG21  | 1.94                     | 0.50              |
| 14:CN:18:ASP:OD2  | 14:CN:18:ASP:N     | 2.45                     | 0.50              |
| 49:D1:5:ILE:HG22  | 49:D1:28:ARG:NH1   | 2.27                     | 0.50              |
| 50:D2:43:THR:O    | 50:D2:44:VAL:HB    | 2.11                     | 0.50              |
| 22:DA:1524:G:H2'  | 22:DA:1524:G:N3    | 2.26                     | 0.50              |
| 22:DA:2583:G:H2'  | 22:DA:2584:U:O4'   | 2.11                     | 0.50              |
| 22:DA:583:G:C5    | 22:DA:584:C:C4     | 3.00                     | 0.50              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:DA:915:C:C4    | 22:DA:916:G:C5    | 3.00                     | 0.50              |
| 24:DC:230:HIS:ND1 | 24:DC:231:PRO:HD2 | 2.27                     | 0.50              |
| 30:DI:77:ALA:HA   | 30:DI:80:LEU:HD12 | 1.93                     | 0.50              |
| 32:DK:118:LEU:O   | 32:DK:119:ALA:HB3 | 2.12                     | 0.50              |
| 33:DL:68:SER:O    | 33:DL:69:ARG:HB2  | 2.12                     | 0.50              |
| 41:DT:3:ARG:CZ    | 41:DT:5:GLU:OE1   | 2.60                     | 0.50              |
| 22:DA:396:G:H5''  | 45:DX:13:VAL:HG21 | 1.93                     | 0.50              |
| 45:DX:17:ASN:HB2  | 45:DX:25:THR:HB   | 1.94                     | 0.50              |
| 1:AA:988:G:C6     | 1:AA:989:U:C4     | 3.00                     | 0.50              |
| 8:AH:51:VAL:CG2   | 8:AH:51:VAL:O     | 2.59                     | 0.50              |
| 9:AI:57:MET:C     | 9:AI:59:GLU:H     | 2.15                     | 0.50              |
| 1:AA:1060:U:H4'   | 10:AJ:53:ILE:HG23 | 1.94                     | 0.50              |
| 17:AQ:16:LYS:O    | 17:AQ:17:MET:HE3  | 2.11                     | 0.50              |
| 20:AT:56:PRO:O    | 20:AT:60:ARG:HB2  | 2.12                     | 0.50              |
| 22:BA:1452:G:H2'  | 22:BA:1457:U:O4   | 2.12                     | 0.50              |
| 22:BA:1717:A:H2'  | 22:BA:1718:G:O4'  | 2.12                     | 0.50              |
| 22:BA:1829:A:O2'  | 24:BC:15:HIS:CD2  | 2.65                     | 0.50              |
| 22:BA:1832:C:N4   | 22:BA:1833:C:C5   | 2.80                     | 0.50              |
| 22:BA:2024:G:OP2  | 22:BA:2034:U:H4'  | 2.11                     | 0.50              |
| 22:BA:2064:C:H2'  | 22:BA:2065:C:C6   | 2.47                     | 0.50              |
| 22:BA:2414:G:C2'  | 22:BA:2415:G:H5'  | 2.42                     | 0.50              |
| 22:BA:274:C:C4    | 22:BA:275:C:C4    | 3.00                     | 0.50              |
| 24:BC:141:VAL:CG1 | 24:BC:190:ALA:HB1 | 2.42                     | 0.50              |
| 25:BD:177:VAL:CG2 | 25:BD:177:VAL:O   | 2.60                     | 0.50              |
| 29:BH:14:SER:HG   | 29:BH:17:ASP:CG   | 2.13                     | 0.50              |
| 43:BV:1:MET:SD    | 43:BV:1:MET:C     | 2.91                     | 0.50              |
| 1:CA:1197:A:H2'   | 1:CA:1198:G:H5'   | 1.92                     | 0.50              |
| 1:CA:1364:U:O2    | 1:CA:1364:U:C2'   | 2.60                     | 0.50              |
| 1:CA:1376:U:O4    | 7:CG:10:ARG:NH1   | 2.45                     | 0.50              |
| 1:CA:32:A:C2      | 1:CA:33:A:C6      | 2.99                     | 0.50              |
| 3:CC:64:ILE:HG12  | 3:CC:66:VAL:HG23  | 1.94                     | 0.50              |
| 19:CS:40:ILE:HA   | 19:CS:44:MET:SD   | 2.52                     | 0.50              |
| 20:CT:68:HIS:C    | 20:CT:69:LYS:HG3  | 2.32                     | 0.50              |
| 20:CT:74:ARG:O    | 20:CT:78:ASN:ND2  | 2.44                     | 0.50              |
| 48:D0:54:VAL:O    | 48:D0:55:ILE:HB   | 2.12                     | 0.50              |
| 22:DA:1257:C:C4   | 22:DA:1258:U:C4   | 2.99                     | 0.50              |
| 22:DA:1288:G:C5   | 22:DA:1327:A:C2   | 3.00                     | 0.50              |
| 22:DA:1378:A:C4'  | 22:DA:1379:U:OP1  | 2.59                     | 0.50              |
| 22:DA:247:G:N7    | 22:DA:249:C:C2    | 2.80                     | 0.50              |
| 22:DA:1662:U:O2   | 22:DA:2687:U:H5'' | 2.12                     | 0.50              |
| 22:DA:289:G:H2'   | 22:DA:290:U:O4'   | 2.12                     | 0.50              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 22:DA:36:G:N1      | 22:DA:445:C:C4    | 2.79                     | 0.50              |
| 22:DA:694:U:C3'    | 22:DA:695:G:C5'   | 2.89                     | 0.50              |
| 22:DA:945:A:C5     | 22:DA:2448:A:C2   | 2.99                     | 0.50              |
| 25:DD:15:PHE:CE2   | 37:DP:78:SER:HA   | 2.47                     | 0.50              |
| 33:DL:78:ARG:HB3   | 33:DL:113:ALA:CB  | 2.42                     | 0.50              |
| 38:DQ:98:ILE:HG22  | 38:DQ:106:PHE:HB2 | 1.94                     | 0.50              |
| 39:DR:68:ARG:HB3   | 39:DR:90:ARG:HG2  | 1.93                     | 0.50              |
| 1:AA:1399:C:C4     | 1:AA:1502:A:N1    | 2.80                     | 0.50              |
| 1:AA:233:C:H2'     | 1:AA:234:C:H6     | 1.77                     | 0.50              |
| 1:AA:374:A:N1      | 1:AA:390:U:O2'    | 2.43                     | 0.50              |
| 11:AK:16:VAL:O     | 11:AK:17:SER:OG   | 2.25                     | 0.50              |
| 13:AM:11:ASP:O     | 13:AM:12:HIS:HB2  | 2.11                     | 0.50              |
| 17:AQ:16:LYS:CG    | 17:AQ:16:LYS:O    | 2.59                     | 0.50              |
| 21:AU:20:LYS:N     | 21:AU:20:LYS:HE2  | 2.27                     | 0.50              |
| 22:BA:586:A:C2     | 22:BA:1254:A:C2   | 3.00                     | 0.50              |
| 22:BA:2243:U:H2'   | 22:BA:2244:U:C6   | 2.47                     | 0.50              |
| 22:BA:437:U:H2'    | 22:BA:438:G:C8    | 2.46                     | 0.50              |
| 27:BF:21:ASN:O     | 27:BF:21:ASN:CG   | 2.50                     | 0.50              |
| 27:BF:8:TYR:HA     | 27:BF:12:VAL:CG2  | 2.41                     | 0.50              |
| 29:BH:43:ASN:O     | 29:BH:46:PHE:HB3  | 2.12                     | 0.50              |
| 30:BI:105:GLN:O    | 30:BI:106:LEU:HB2 | 2.12                     | 0.50              |
| 41:BT:1:MET:O      | 41:BT:2:ILE:CG1   | 2.60                     | 0.50              |
| 42:BU:20:GLY:O     | 42:BU:21:LYS:O    | 2.29                     | 0.50              |
| 1:CA:1072:G:OP1    | 5:CE:62:LYS:NZ    | 2.44                     | 0.50              |
| 1:CA:1089:G:C5     | 1:CA:1090:U:C5    | 3.00                     | 0.50              |
| 1:CA:1279:G:OP2    | 10:CJ:11:LYS:NZ   | 2.42                     | 0.50              |
| 1:CA:1347:G:O2'    | 1:CA:1348:U:P     | 2.70                     | 0.50              |
| 1:CA:147:G:N2      | 1:CA:148:G:C6     | 2.80                     | 0.50              |
| 1:CA:380:G:N2      | 1:CA:383:A:OP2    | 2.37                     | 0.50              |
| 1:CA:963:G:C2'     | 1:CA:964:A:H5'    | 2.42                     | 0.50              |
| 11:CK:110:ILE:HG22 | 21:CU:17:ARG:NH1  | 2.27                     | 0.50              |
| 12:CL:3:THR:CB     | 12:CL:6:GLN:HG3   | 2.42                     | 0.50              |
| 17:CQ:69:LYS:C     | 17:CQ:70:THR:OG1  | 2.49                     | 0.50              |
| 20:CT:60:ARG:O     | 20:CT:64:LYS:HB2  | 2.12                     | 0.50              |
| 22:DA:1026:G:H1'   | 22:DA:1134:A:C2   | 2.46                     | 0.50              |
| 22:DA:1352:U:C5    | 22:DA:1377:G:C5   | 2.99                     | 0.50              |
| 22:DA:1627:G:N2    | 22:DA:1628:G:C5   | 2.80                     | 0.50              |
| 22:DA:1731:G:C6    | 22:DA:1733:G:C5   | 3.00                     | 0.50              |
| 22:DA:1754:A:N6    | 22:DA:1755:A:N6   | 2.60                     | 0.50              |
| 22:DA:1998:A:OP2   | 25:DD:141:ARG:NH2 | 2.45                     | 0.50              |
| 22:DA:2223:G:H2'   | 22:DA:2224:G:H5'  | 1.94                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:DA:270:A:C2     | 22:DA:369:U:H4'    | 2.46                     | 0.50              |
| 22:DA:419:U:N3     | 22:DA:420:C:C5     | 2.80                     | 0.50              |
| 22:DA:533:G:H5'    | 38:DQ:24:TYR:CE2   | 2.47                     | 0.50              |
| 22:DA:634:C:P      | 33:DL:70:LYS:HE2   | 2.52                     | 0.50              |
| 22:DA:89:A:C2      | 22:DA:90:U:C2      | 3.00                     | 0.50              |
| 23:DB:37:C:C5      | 23:DB:38:C:C4      | 3.00                     | 0.50              |
| 24:DC:18:LYS:O     | 24:DC:19:VAL:CB    | 2.59                     | 0.50              |
| 25:DD:106:LYS:HA   | 25:DD:175:LEU:O    | 2.12                     | 0.50              |
| 31:DJ:142:ILE:OXT  | 31:DJ:142:ILE:HG23 | 2.11                     | 0.50              |
| 33:DL:68:SER:O     | 33:DL:69:ARG:CB    | 2.58                     | 0.50              |
| 43:DV:9:ARG:HG2    | 43:DV:41:GLU:HB3   | 1.94                     | 0.50              |
| 1:AA:1315:U:C4     | 1:AA:1316:G:C6     | 3.00                     | 0.49              |
| 1:AA:223:A:C6      | 1:AA:224:U:C4      | 2.99                     | 0.49              |
| 1:AA:453:G:H2'     | 1:AA:454:G:C8      | 2.47                     | 0.49              |
| 1:AA:645:G:N7      | 57:AA:1749:HOH:O   | 2.35                     | 0.49              |
| 1:AA:844:G:N3      | 1:AA:845:A:N7      | 2.60                     | 0.49              |
| 3:AC:145:GLY:O     | 3:AC:146:ALA:O     | 2.30                     | 0.49              |
| 5:AE:56:VAL:O      | 5:AE:60:ILE:HG23   | 2.11                     | 0.49              |
| 6:AF:9:MET:HE2     | 18:AR:65:LEU:HD22  | 1.93                     | 0.49              |
| 9:AI:30:ILE:HA     | 9:AI:65:ILE:O      | 2.12                     | 0.49              |
| 10:AJ:35:GLN:HG3   | 10:AJ:77:VAL:HB    | 1.93                     | 0.49              |
| 12:AL:107:VAL:HG23 | 12:AL:117:TYR:HB3  | 1.94                     | 0.49              |
| 16:AP:38:PHE:CZ    | 16:AP:51:ARG:HB2   | 2.47                     | 0.49              |
| 21:AU:40:LYS:N     | 21:AU:41:PRO:CD    | 2.75                     | 0.49              |
| 1:AA:723:U:O5'     | 21:AU:49:LYS:HG2   | 2.11                     | 0.49              |
| 53:B5:50:ILE:HG22  | 53:B5:51:ASP:H     | 1.77                     | 0.49              |
| 22:BA:1316:U:C2    | 22:BA:1337:G:N2    | 2.80                     | 0.49              |
| 22:BA:1439:A:N3    | 22:BA:1553:A:C6    | 2.80                     | 0.49              |
| 22:BA:1926:U:O2    | 22:BA:1926:U:H2'   | 2.12                     | 0.49              |
| 22:BA:2057:G:OP2   | 57:BA:3492:HOH:O   | 2.18                     | 0.49              |
| 22:BA:2298:A:C4    | 22:BA:2321:U:C5    | 2.99                     | 0.49              |
| 22:BA:2636:C:H2'   | 22:BA:2637:U:C6    | 2.47                     | 0.49              |
| 22:BA:1297:C:OP1   | 22:BA:2710:C:H4'   | 2.12                     | 0.49              |
| 22:BA:2771:C:H2'   | 22:BA:2772:C:H6    | 1.77                     | 0.49              |
| 22:BA:684:G:OP1    | 50:B2:21:ARG:NH1   | 2.45                     | 0.49              |
| 24:BC:247:PRO:HD2  | 24:BC:248:TRP:CZ3  | 2.47                     | 0.49              |
| 25:BD:12:THR:CG2   | 37:BP:9:GLU:OE2    | 2.59                     | 0.49              |
| 27:BF:63:GLN:OE1   | 27:BF:95:ARG:HD2   | 2.12                     | 0.49              |
| 29:BH:99:ILE:O     | 29:BH:99:ILE:HG22  | 2.12                     | 0.49              |
| 34:BM:66:ARG:NH1   | 34:BM:104:GLU:OE1  | 2.45                     | 0.49              |
| 1:CA:109:A:C6      | 1:CA:327:A:C5      | 3.00                     | 0.49              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:CA:74:A:C2      | 1:CA:75:G:C5       | 3.00                     | 0.49              |
| 1:CA:844:G:N3     | 1:CA:844:G:H2'     | 2.27                     | 0.49              |
| 2:CB:219:ALA:O    | 2:CB:220:THR:CB    | 2.60                     | 0.49              |
| 3:CC:57:ILE:HG13  | 3:CC:66:VAL:HG22   | 1.93                     | 0.49              |
| 4:CD:116:GLN:HG3  | 4:CD:120:HIS:CE1   | 2.47                     | 0.49              |
| 9:CI:30:ILE:HA    | 9:CI:65:ILE:HG13   | 1.94                     | 0.49              |
| 10:CJ:33:GLY:HA3  | 10:CJ:83:THR:HB    | 1.93                     | 0.49              |
| 48:D0:31:ASP:OD1  | 48:D0:48:TYR:HB3   | 2.12                     | 0.49              |
| 52:D4:20:ASP:OD2  | 57:D4:201:HOH:O    | 2.20                     | 0.49              |
| 22:DA:1082:U:H5'  | 30:DI:119:GLY:HA2  | 1.94                     | 0.49              |
| 22:DA:132:G:N2    | 22:DA:148:U:C2     | 2.80                     | 0.49              |
| 22:DA:158:U:C4    | 22:DA:159:G:C5     | 2.99                     | 0.49              |
| 22:DA:1667:G:N3   | 22:DA:1991:U:C5    | 2.80                     | 0.49              |
| 22:DA:532:A:N7    | 22:DA:2021:C:H2'   | 2.26                     | 0.49              |
| 22:DA:2478:A:N7   | 22:DA:2529:G:C6    | 2.80                     | 0.49              |
| 22:DA:681:G:C4    | 22:DA:682:G:C8     | 3.00                     | 0.49              |
| 22:DA:695:G:C5    | 22:DA:768:G:C6     | 3.00                     | 0.49              |
| 23:DB:109:A:C6    | 23:DB:110:C:C4     | 2.99                     | 0.49              |
| 24:DC:178:SER:O   | 24:DC:271:ARG:HB2  | 2.12                     | 0.49              |
| 24:DC:87:ARG:NH1  | 24:DC:87:ARG:HB3   | 2.27                     | 0.49              |
| 29:DH:127:GLU:HG3 | 29:DH:145:ASN:HA   | 1.93                     | 0.49              |
| 30:DI:97:LYS:HD2  | 30:DI:97:LYS:N     | 2.27                     | 0.49              |
| 34:DM:53:MET:HG3  | 34:DM:54:THR:N     | 2.27                     | 0.49              |
| 37:DP:24:ASP:O    | 37:DP:25:THR:OG1   | 2.28                     | 0.49              |
| 37:DP:99:TYR:CE2  | 37:DP:100:LEU:CD2  | 2.95                     | 0.49              |
| 1:AA:1144:G:N1    | 1:AA:1145:A:C2     | 2.80                     | 0.49              |
| 1:AA:1296:C:H4'   | 1:AA:1302:C:C5     | 2.47                     | 0.49              |
| 1:AA:22:G:H2'     | 1:AA:23:C:H6       | 1.77                     | 0.49              |
| 1:AA:451:A:H4'    | 1:AA:452:A:O4'     | 2.12                     | 0.49              |
| 2:AB:24:ASN:O     | 2:AB:27:MET:N      | 2.42                     | 0.49              |
| 13:AM:14:HIS:HB2  | 13:AM:17:ILE:HD13  | 1.94                     | 0.49              |
| 14:AN:43:ASN:C    | 14:AN:45:VAL:N     | 2.65                     | 0.49              |
| 1:AA:261:U:C5     | 20:AT:74:ARG:NH1   | 2.79                     | 0.49              |
| 22:BA:1734:G:H2'  | 22:BA:1735:A:C8    | 2.48                     | 0.49              |
| 22:BA:2415:G:H2'  | 22:BA:2416:C:H6    | 1.75                     | 0.49              |
| 22:BA:1783:A:N1   | 22:BA:2587:A:H2'   | 2.27                     | 0.49              |
| 22:BA:2619:C:OP1  | 25:BD:157:LYS:HE2  | 2.12                     | 0.49              |
| 22:BA:348:A:H2'   | 22:BA:349:U:O4'    | 2.11                     | 0.49              |
| 22:BA:510:C:OP1   | 22:BA:512:G:O6     | 2.30                     | 0.49              |
| 31:BJ:77:HIS:HA   | 31:BJ:83:GLY:O     | 2.12                     | 0.49              |
| 34:BM:57:VAL:HG12 | 34:BM:112:LEU:HD23 | 1.94                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 38:BQ:89:GLU:H    | 39:BR:49:ILE:HD12 | 1.76                     | 0.49              |
| 45:BX:11:ARG:HB2  | 45:BX:12:PRO:CD   | 2.41                     | 0.49              |
| 46:BY:20:ASN:O    | 46:BY:24:GLU:HB2  | 2.11                     | 0.49              |
| 1:CA:1134:G:C6    | 1:CA:1135:U:C2    | 2.99                     | 0.49              |
| 1:CA:1252:A:H2'   | 1:CA:1253:G:O4'   | 2.12                     | 0.49              |
| 1:CA:183:C:O2'    | 1:CA:184:G:C5'    | 2.61                     | 0.49              |
| 1:CA:29:U:H4'     | 1:CA:295:C:O3'    | 2.12                     | 0.49              |
| 1:CA:216:U:H5''   | 1:CA:464:U:H4'    | 1.93                     | 0.49              |
| 4:CD:22:LYS:C     | 4:CD:24:GLY:N     | 2.64                     | 0.49              |
| 6:CF:32:ALA:O     | 6:CF:33:GLU:C     | 2.51                     | 0.49              |
| 6:CF:86:ARG:HH11  | 6:CF:86:ARG:HG2   | 1.77                     | 0.49              |
| 8:CH:75:ILE:HD13  | 8:CH:129:VAL:HG22 | 1.94                     | 0.49              |
| 9:CI:63:LEU:O     | 9:CI:63:LEU:HG    | 2.12                     | 0.49              |
| 1:CA:1179:A:OP2   | 9:CI:99:ARG:NH2   | 2.45                     | 0.49              |
| 6:CF:59:TYR:HE2   | 18:CR:67:LEU:CD2  | 2.25                     | 0.49              |
| 21:CU:4:ILE:HG22  | 21:CU:4:ILE:O     | 2.13                     | 0.49              |
| 48:D0:20:ASP:N    | 48:D0:20:ASP:OD2  | 2.44                     | 0.49              |
| 50:D2:15:SER:OG   | 50:D2:16:HIS:CE1  | 2.65                     | 0.49              |
| 22:DA:86:G:O2'    | 22:DA:104:A:H4'   | 2.12                     | 0.49              |
| 22:DA:1299:G:H5'' | 22:DA:1300:G:H5'' | 1.93                     | 0.49              |
| 22:DA:1355:G:C2   | 22:DA:1356:G:C8   | 3.00                     | 0.49              |
| 22:DA:1476:U:H1'  | 22:DA:1732:C:O2   | 2.12                     | 0.49              |
| 22:DA:2127:G:N3   | 22:DA:2162:G:C8   | 2.80                     | 0.49              |
| 22:DA:591:U:H1'   | 51:D3:2:PRO:HD2   | 1.94                     | 0.49              |
| 22:DA:776:G:N7    | 22:DA:793:A:C4    | 2.81                     | 0.49              |
| 24:DC:246:THR:O   | 24:DC:248:TRP:N   | 2.45                     | 0.49              |
| 25:DD:148:GLN:N   | 25:DD:148:GLN:OE1 | 2.45                     | 0.49              |
| 27:DF:16:LEU:HD11 | 27:DF:169:LEU:CD1 | 2.43                     | 0.49              |
| 22:DA:1076:C:O2'  | 30:DI:93:PRO:HD2  | 2.12                     | 0.49              |
| 22:DA:1654:A:OP1  | 35:DN:1:MET:HA    | 2.11                     | 0.49              |
| 46:DY:50:VAL:O    | 46:DY:54:LYS:HG3  | 2.12                     | 0.49              |
| 1:AA:1255:G:O2'   | 1:AA:1258:G:N3    | 2.43                     | 0.49              |
| 1:AA:1277:C:O2'   | 1:AA:1279:G:C8    | 2.63                     | 0.49              |
| 1:AA:1347:G:N2    | 1:AA:1373:G:H2'   | 2.27                     | 0.49              |
| 1:AA:142:G:H2'    | 1:AA:142:G:N3     | 2.27                     | 0.49              |
| 1:AA:255:G:C6     | 1:AA:256:U:C4     | 3.01                     | 0.49              |
| 1:AA:49:U:C2      | 1:AA:361:G:N2     | 2.81                     | 0.49              |
| 1:AA:651:C:C2'    | 1:AA:652:U:O5'    | 2.60                     | 0.49              |
| 3:AC:193:TYR:CD2  | 3:AC:193:TYR:N    | 2.79                     | 0.49              |
| 5:AE:74:VAL:HG11  | 5:AE:144:LEU:HB3  | 1.93                     | 0.49              |
| 19:AS:58:VAL:HG11 | 19:AS:75:ALA:HA   | 1.95                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 53:B5:65:LEU:O    | 53:B5:67:HIS:N    | 2.44                     | 0.49              |
| 22:BA:1026:G:H2'  | 22:BA:1027:A:C8   | 2.46                     | 0.49              |
| 22:BA:1209:U:O2'  | 22:BA:1237:A:N1   | 2.42                     | 0.49              |
| 22:BA:2469:A:H4'  | 34:BM:55:ARG:HH12 | 1.76                     | 0.49              |
| 22:BA:2662:A:H5'' | 22:BA:2663:G:OP2  | 2.12                     | 0.49              |
| 22:BA:393:C:H2'   | 22:BA:394:C:H6    | 1.77                     | 0.49              |
| 22:BA:478:A:C6    | 22:BA:480:A:C6    | 3.01                     | 0.49              |
| 22:BA:674:G:H1'   | 26:BE:69:ARG:HD3  | 1.94                     | 0.49              |
| 26:BE:23:PHE:HB2  | 26:BE:111:GLU:HG3 | 1.94                     | 0.49              |
| 29:BH:86:ASP:O    | 29:BH:87:GLU:HB2  | 2.11                     | 0.49              |
| 31:BJ:23:LYS:O    | 31:BJ:63:ALA:HB3  | 2.12                     | 0.49              |
| 37:BP:26:VAL:CG1  | 37:BP:47:VAL:HG23 | 2.43                     | 0.49              |
| 40:BS:84:ARG:HB2  | 40:BS:96:ILE:HD11 | 1.94                     | 0.49              |
| 1:CA:1002:G:C2    | 1:CA:1003:G:H1'   | 2.47                     | 0.49              |
| 1:CA:1000:A:C2    | 1:CA:1041:G:C2    | 3.00                     | 0.49              |
| 1:CA:1315:U:O2'   | 1:CA:1360:A:N3    | 2.34                     | 0.49              |
| 1:CA:1409:C:H4'   | 22:DA:1915:U:O4   | 2.12                     | 0.49              |
| 1:CA:1412:C:H2'   | 1:CA:1413:A:C8    | 2.47                     | 0.49              |
| 1:CA:213:G:C8     | 1:CA:214:C:C5     | 3.00                     | 0.49              |
| 1:CA:321:A:C8     | 1:CA:328:C:C2     | 3.00                     | 0.49              |
| 1:CA:771:G:C4     | 1:CA:809:G:N2     | 2.80                     | 0.49              |
| 5:CE:150:PRO:HA   | 8:CH:99:LEU:CD2   | 2.41                     | 0.49              |
| 9:CI:88:MET:HA    | 9:CI:92:GLU:OE2   | 2.12                     | 0.49              |
| 22:DA:1356:G:C2   | 22:DA:1357:C:H1'  | 2.47                     | 0.49              |
| 22:DA:1530:G:N2   | 22:DA:1542:U:O2   | 2.45                     | 0.49              |
| 22:DA:2454:G:H1'  | 57:DA:3531:HOH:O  | 2.12                     | 0.49              |
| 22:DA:411:G:OP1   | 22:DA:2407:A:OP2  | 2.29                     | 0.49              |
| 22:DA:547:A:H3'   | 22:DA:548:G:C5'   | 2.42                     | 0.49              |
| 22:DA:579:G:N2    | 22:DA:1262:A:C4   | 2.80                     | 0.49              |
| 22:DA:655:A:H4'   | 22:DA:656:G:OP1   | 2.11                     | 0.49              |
| 22:DA:971:G:C2    | 22:DA:972:A:H1'   | 2.47                     | 0.49              |
| 24:DC:57:GLY:HA3  | 24:DC:213:TRP:HA  | 1.94                     | 0.49              |
| 30:DI:22:PRO:HB2  | 30:DI:23:PRO:HD3  | 1.95                     | 0.49              |
| 33:DL:108:ALA:HB3 | 33:DL:125:LEU:HG  | 1.94                     | 0.49              |
| 35:DN:36:THR:HG23 | 35:DN:41:ALA:HB2  | 1.95                     | 0.49              |
| 42:DU:7:ARG:CG    | 42:DU:8:ASP:N     | 2.75                     | 0.49              |
| 41:DT:14:PRO:HD2  | 46:DY:33:ALA:HB1  | 1.93                     | 0.49              |
| 47:DZ:3:LYS:O     | 47:DZ:4:THR:HG22  | 2.12                     | 0.49              |
| 1:AA:406:G:O5'    | 4:AD:5:LEU:HD11   | 2.13                     | 0.49              |
| 4:AD:190:ASP:O    | 4:AD:191:LEU:O    | 2.30                     | 0.49              |
| 4:AD:65:TYR:CG    | 4:AD:94:LEU:HD22  | 2.48                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 9:AI:26:GLY:CA    | 9:AI:59:GLU:HA    | 2.42                     | 0.49              |
| 9:AI:40:GLY:O     | 9:AI:41:ARG:HB2   | 2.10                     | 0.49              |
| 12:AL:50:ARG:NH1  | 12:AL:89:ASP:OD1  | 2.35                     | 0.49              |
| 13:AM:29:ARG:O    | 13:AM:33:ILE:HG12 | 2.12                     | 0.49              |
| 1:AA:254:G:OP1    | 17:AQ:69:LYS:O    | 2.30                     | 0.49              |
| 19:AS:10:PHE:CG   | 19:AS:11:ILE:N    | 2.80                     | 0.49              |
| 19:AS:34:TRP:O    | 19:AS:36:ARG:HG3  | 2.13                     | 0.49              |
| 22:BA:1239:G:H2'  | 22:BA:1240:U:O4'  | 2.12                     | 0.49              |
| 22:BA:1377:G:H5'' | 22:BA:1378:A:OP2  | 2.12                     | 0.49              |
| 22:BA:1487:U:C2   | 22:BA:1503:A:C2   | 2.99                     | 0.49              |
| 22:BA:1952:A:C6   | 22:BA:1953:A:N1   | 2.80                     | 0.49              |
| 22:BA:2077:A:O2'  | 22:BA:2078:C:H5'  | 2.12                     | 0.49              |
| 22:BA:236:C:O2'   | 22:BA:237:C:H5'   | 2.13                     | 0.49              |
| 22:BA:825:A:H4'   | 22:BA:2428:G:C5   | 2.47                     | 0.49              |
| 22:BA:2582:G:OP2  | 22:BA:2583:G:OP2  | 2.31                     | 0.49              |
| 22:BA:2665:A:C2   | 22:BA:2666:C:C6   | 3.00                     | 0.49              |
| 22:BA:2808:G:N2   | 22:BA:2891:U:C6   | 2.80                     | 0.49              |
| 22:BA:601:C:O2    | 22:BA:605:G:H4'   | 2.13                     | 0.49              |
| 22:BA:783:A:H8    | 22:BA:784:G:H4'   | 1.76                     | 0.49              |
| 23:BB:2:G:C2      | 23:BB:119:A:C2    | 3.00                     | 0.49              |
| 22:BA:1791:A:O2'  | 24:BC:206:GLY:HA2 | 2.13                     | 0.49              |
| 30:BI:106:LEU:HA  | 30:BI:109:ILE:HB  | 1.94                     | 0.49              |
| 37:BP:51:ARG:O    | 37:BP:57:SER:HA   | 2.12                     | 0.49              |
| 22:BA:1340:U:OP1  | 41:BT:19:LYS:NZ   | 2.45                     | 0.49              |
| 1:CA:1004:A:C2    | 1:CA:1026:G:N3    | 2.80                     | 0.49              |
| 1:CA:101:A:C4     | 1:CA:102:G:C8     | 3.01                     | 0.49              |
| 1:CA:1124:G:N2    | 1:CA:1127:G:N2    | 2.59                     | 0.49              |
| 1:CA:1162:C:C2    | 1:CA:1175:G:N2    | 2.80                     | 0.49              |
| 1:CA:927:G:N2     | 1:CA:1391:U:H1'   | 2.28                     | 0.49              |
| 1:CA:145:G:N2     | 1:CA:146:G:C4     | 2.81                     | 0.49              |
| 1:CA:666:G:C6     | 1:CA:741:G:C6     | 3.01                     | 0.49              |
| 4:CD:9:LEU:HD11   | 4:CD:29:ASP:OD1   | 2.12                     | 0.49              |
| 9:CI:50:GLN:N     | 9:CI:51:PRO:HD2   | 2.28                     | 0.49              |
| 22:DA:1097:U:H1'  | 30:DI:9:VAL:HG11  | 1.94                     | 0.49              |
| 22:DA:1187:G:N7   | 57:DA:3574:HOH:O  | 2.35                     | 0.49              |
| 22:DA:1231:U:H2'  | 22:DA:1232:G:H8   | 1.76                     | 0.49              |
| 22:DA:1317:G:H2'  | 22:DA:1318:U:O4'  | 2.12                     | 0.49              |
| 22:DA:1464:G:C2   | 22:DA:1465:G:C4   | 3.01                     | 0.49              |
| 22:DA:1627:G:N2   | 22:DA:1628:G:N7   | 2.60                     | 0.49              |
| 22:DA:2223:G:C2'  | 22:DA:2224:G:H5'  | 2.41                     | 0.49              |
| 22:DA:2331:G:N2   | 22:DA:2385:C:C2   | 2.80                     | 0.49              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:DA:2518:A:H2'   | 22:DA:2518:A:N3    | 2.26                     | 0.49              |
| 22:DA:810:U:C4     | 33:DL:30:THR:HA    | 2.47                     | 0.49              |
| 22:DA:931:U:OP1    | 47:DZ:30:ARG:NH1   | 2.46                     | 0.49              |
| 23:DB:42:C:O2'     | 27:DF:63:GLN:NE2   | 2.45                     | 0.49              |
| 23:DB:40:U:C2      | 23:DB:44:G:OP2     | 2.65                     | 0.49              |
| 26:DE:170:ARG:CZ   | 26:DE:176:ASP:OD1  | 2.61                     | 0.49              |
| 29:DH:81:ALA:C     | 29:DH:149:GLU:HB3  | 2.33                     | 0.49              |
| 39:DR:78:ARG:CB    | 39:DR:83:TYR:CD1   | 2.94                     | 0.49              |
| 23:DB:76:G:O2'     | 43:DV:78:GLN:OE1   | 2.16                     | 0.49              |
| 45:DX:40:VAL:HG22  | 45:DX:45:ARG:O     | 2.13                     | 0.49              |
| 1:AA:104:G:C2      | 1:AA:105:G:C5      | 3.01                     | 0.49              |
| 1:AA:119:A:C2      | 1:AA:240:G:C8      | 3.01                     | 0.49              |
| 1:AA:1307:U:H2'    | 1:AA:1308:U:C6     | 2.48                     | 0.49              |
| 1:AA:1457:G:H2'    | 1:AA:1458:G:O4'    | 2.12                     | 0.49              |
| 1:AA:32:A:N3       | 1:AA:32:A:H2'      | 2.27                     | 0.49              |
| 1:AA:383:A:C5      | 1:AA:384:G:H1'     | 2.48                     | 0.49              |
| 4:AD:99:ASP:OD2    | 4:AD:115:ARG:NH2   | 2.45                     | 0.49              |
| 4:AD:34:ILE:O      | 4:AD:35:GLU:CB     | 2.60                     | 0.49              |
| 4:AD:35:GLU:O      | 4:AD:38:PRO:HD3    | 2.13                     | 0.49              |
| 9:AI:112:GLU:OE2   | 9:AI:115:LYS:NZ    | 2.45                     | 0.49              |
| 10:AJ:49:PHE:CD1   | 10:AJ:49:PHE:N     | 2.81                     | 0.49              |
| 22:BA:1061:U:H3'   | 22:BA:1062:G:H5'   | 1.94                     | 0.49              |
| 22:BA:108:G:C6     | 22:BA:109:C:C4     | 3.01                     | 0.49              |
| 22:BA:1153:C:H2'   | 22:BA:1154:G:O4'   | 2.13                     | 0.49              |
| 22:BA:1168:G:H2'   | 22:BA:1169:A:O4'   | 2.13                     | 0.49              |
| 22:BA:1747:U:O2'   | 22:BA:1748:C:H5'   | 2.13                     | 0.49              |
| 22:BA:2032:G:C8    | 57:BA:3537:HOH:O   | 2.64                     | 0.49              |
| 22:BA:2302:U:O2'   | 22:BA:2303:G:H5'   | 2.12                     | 0.49              |
| 26:BE:104:ALA:O    | 26:BE:108:ILE:HG23 | 2.13                     | 0.49              |
| 27:BF:135:GLN:OE1  | 27:BF:135:GLN:N    | 2.43                     | 0.49              |
| 27:BF:158:THR:HG22 | 27:BF:160:ALA:HB3  | 1.94                     | 0.49              |
| 41:BT:28:ASN:HD21  | 41:BT:91:GLN:HB2   | 1.78                     | 0.49              |
| 42:BU:96:PHE:O     | 42:BU:100:SER:HA   | 2.12                     | 0.49              |
| 1:CA:1171:A:C2     | 1:CA:1172:C:C2     | 3.00                     | 0.49              |
| 1:CA:1201:A:H1'    | 1:CA:1202:U:OP2    | 2.13                     | 0.49              |
| 1:CA:1363:A:N3     | 1:CA:1363:A:H2'    | 2.27                     | 0.49              |
| 1:CA:1502:A:H5'    | 1:CA:1504:G:N7     | 2.27                     | 0.49              |
| 1:CA:307:C:H5''    | 1:CA:308:C:OP2     | 2.12                     | 0.49              |
| 4:CD:168:PRO:O     | 4:CD:170:TRP:N     | 2.46                     | 0.49              |
| 6:CF:4:TYR:CD2     | 6:CF:71:ILE:HG21   | 2.48                     | 0.49              |
| 6:CF:78:PHE:N      | 6:CF:78:PHE:CD2    | 2.80                     | 0.49              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 17:CQ:16:LYS:C    | 17:CQ:17:MET:SD    | 2.91                     | 0.49              |
| 22:DA:1097:U:C4   | 22:DA:1098:A:H1'   | 2.48                     | 0.49              |
| 22:DA:1262:A:C6   | 22:DA:1263:U:N3    | 2.80                     | 0.49              |
| 22:DA:1330:C:H2'  | 22:DA:1331:G:O5'   | 2.11                     | 0.49              |
| 22:DA:1343:G:C6   | 22:DA:1344:U:C4    | 3.01                     | 0.49              |
| 22:DA:1366:A:OP1  | 45:DX:2:SER:OG     | 2.25                     | 0.49              |
| 22:DA:1360:G:C6   | 22:DA:1372:U:C2    | 3.00                     | 0.49              |
| 22:DA:1648:U:H2'  | 22:DA:1649:G:O4'   | 2.12                     | 0.49              |
| 22:DA:1847:A:HO2' | 22:DA:1848:A:P     | 2.35                     | 0.49              |
| 22:DA:189:G:C4    | 22:DA:205:G:N2     | 2.80                     | 0.49              |
| 22:DA:2066:C:H5'' | 57:DA:3504:HOH:O   | 2.12                     | 0.49              |
| 22:DA:2300:C:C4   | 22:DA:2317:A:C2    | 3.00                     | 0.49              |
| 22:DA:2335:A:C6   | 22:DA:2337:G:H1'   | 2.47                     | 0.49              |
| 22:DA:2602:A:H4'  | 22:DA:2603:G:H5'   | 1.94                     | 0.49              |
| 22:DA:2796:U:C4   | 22:DA:2798:U:O4    | 2.66                     | 0.49              |
| 22:DA:2854:G:N2   | 22:DA:2864:G:C2    | 2.81                     | 0.49              |
| 22:DA:503:A:C2    | 22:DA:506:G:C5     | 3.01                     | 0.49              |
| 22:DA:536:G:C2'   | 22:DA:537:G:H5'    | 2.42                     | 0.49              |
| 22:DA:646:U:H3'   | 22:DA:647:G:C4'    | 2.43                     | 0.49              |
| 22:DA:654:A:N3    | 22:DA:654:A:H3'    | 2.26                     | 0.49              |
| 22:DA:737:C:C2    | 22:DA:738:G:C8     | 3.00                     | 0.49              |
| 22:DA:747:U:C5    | 22:DA:2613:U:C5    | 3.00                     | 0.49              |
| 24:DC:146:MET:HE3 | 24:DC:182:ARG:NH2  | 2.27                     | 0.49              |
| 29:DH:112:LYS:CG  | 29:DH:113:SER:N    | 2.76                     | 0.49              |
| 30:DI:58:VAL:CG1  | 30:DI:59:ILE:H     | 2.26                     | 0.49              |
| 33:DL:93:ASN:O    | 33:DL:95:LEU:N     | 2.42                     | 0.49              |
| 36:DO:78:VAL:HA   | 36:DO:81:ARG:HB2   | 1.94                     | 0.49              |
| 40:DS:70:LYS:O    | 40:DS:107:VAL:HG23 | 2.11                     | 0.49              |
| 1:AA:1014:A:H2'   | 1:AA:1015:G:O4'    | 2.12                     | 0.49              |
| 1:AA:157:U:O2'    | 1:AA:158:G:H5'     | 2.12                     | 0.49              |
| 1:AA:346:G:P      | 32:BK:105:ARG:NH1  | 2.85                     | 0.49              |
| 1:AA:474:G:C2     | 1:AA:475:C:C6      | 3.00                     | 0.49              |
| 1:AA:720:C:H5''   | 18:AR:41:PRO:HA    | 1.95                     | 0.49              |
| 2:AB:213:TYR:O    | 2:AB:217:VAL:HG23  | 2.12                     | 0.49              |
| 2:AB:82:ASP:O     | 2:AB:84:ALA:N      | 2.46                     | 0.49              |
| 4:AD:70:ARG:O     | 4:AD:74:ASN:ND2    | 2.45                     | 0.49              |
| 5:AE:109:GLY:HA2  | 5:AE:112:ARG:HB3   | 1.94                     | 0.49              |
| 6:AF:51:ILE:O     | 6:AF:52:ASN:HB2    | 2.11                     | 0.49              |
| 6:AF:98:GLU:HG3   | 6:AF:99:ALA:N      | 2.28                     | 0.49              |
| 14:AN:46:LEU:HD12 | 14:AN:46:LEU:C     | 2.33                     | 0.49              |
| 19:AS:18:LYS:O    | 19:AS:31:LEU:HD21  | 2.12                     | 0.49              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:BA:1087:G:O2'  | 22:BA:1089:A:O4'   | 2.27                     | 0.49              |
| 22:BA:1403:A:H2'  | 22:BA:1404:C:C6    | 2.48                     | 0.49              |
| 22:BA:1408:G:C6   | 22:BA:1409:U:C4    | 3.01                     | 0.49              |
| 22:BA:1489:C:C2   | 22:BA:1501:G:C2    | 3.00                     | 0.49              |
| 22:BA:1886:U:C2'  | 22:BA:1887:C:H5'   | 2.43                     | 0.49              |
| 22:BA:570:G:H2'   | 22:BA:2030:A:N7    | 2.28                     | 0.49              |
| 22:BA:528:A:H2    | 22:BA:2043:C:H5'   | 1.74                     | 0.49              |
| 22:BA:570:G:H2'   | 22:BA:2030:A:C8    | 2.48                     | 0.49              |
| 26:BE:29:HIS:CE1  | 26:BE:33:VAL:HG21  | 2.47                     | 0.49              |
| 43:BV:89:ILE:HG21 | 43:BV:91:PHE:CZ    | 2.47                     | 0.49              |
| 1:CA:1386:G:N3    | 1:CA:1387:G:C8     | 2.80                     | 0.49              |
| 1:CA:815:A:H4'    | 1:CA:817:C:C4      | 2.47                     | 0.49              |
| 8:CH:86:TYR:CE2   | 8:CH:124:GLU:HB2   | 2.47                     | 0.49              |
| 17:CQ:50:ASN:O    | 17:CQ:51:ASN:C     | 2.51                     | 0.49              |
| 17:CQ:51:ASN:ND2  | 17:CQ:51:ASN:O     | 2.46                     | 0.49              |
| 50:D2:12:ARG:NH2  | 50:D2:44:VAL:CG1   | 2.75                     | 0.49              |
| 22:DA:1965:C:OP1  | 22:DA:1966:A:C2'   | 2.61                     | 0.49              |
| 22:DA:2322:A:H2'  | 22:DA:2323:G:O4'   | 2.12                     | 0.49              |
| 22:DA:2461:A:H1'  | 22:DA:2492:U:C2    | 2.48                     | 0.49              |
| 22:DA:273:G:H2'   | 22:DA:274:C:O4'    | 2.12                     | 0.49              |
| 22:DA:320:A:H4'   | 22:DA:322:A:N7     | 2.28                     | 0.49              |
| 22:DA:39:G:C6     | 22:DA:40:U:O4      | 2.64                     | 0.49              |
| 22:DA:508:A:H3'   | 22:DA:509:C:H5'    | 1.94                     | 0.49              |
| 22:DA:613:A:HO2'  | 22:DA:614:A:P      | 2.31                     | 0.49              |
| 24:DC:141:VAL:CG1 | 24:DC:190:ALA:HB1  | 2.42                     | 0.49              |
| 26:DE:146:VAL:O   | 26:DE:167:VAL:HA   | 2.12                     | 0.49              |
| 27:DF:108:VAL:N   | 27:DF:109:PRO:CD   | 2.76                     | 0.49              |
| 30:DI:9:VAL:HG23  | 30:DI:10:LYS:N     | 2.28                     | 0.49              |
| 32:DK:31:ARG:CB   | 32:DK:32:TYR:CD2   | 2.96                     | 0.49              |
| 33:DL:116:VAL:O   | 33:DL:116:VAL:HG13 | 2.12                     | 0.49              |
| 33:DL:55:MET:SD   | 33:DL:59:ARG:CZ    | 3.01                     | 0.49              |
| 22:DA:1454:C:H5'  | 35:DN:63:ARG:HD3   | 1.94                     | 0.49              |
| 1:AA:929:G:N2     | 1:AA:1389:C:C2     | 2.81                     | 0.49              |
| 1:AA:1442:G:H2'   | 1:AA:1443:C:H6     | 1.77                     | 0.49              |
| 1:AA:259:G:C2     | 1:AA:260:G:H1'     | 2.47                     | 0.49              |
| 1:AA:937:A:N6     | 1:AA:1345:U:O4     | 2.46                     | 0.49              |
| 2:AB:40:ILE:HD13  | 2:AB:40:ILE:N      | 2.27                     | 0.49              |
| 6:AF:35:LYS:HD3   | 6:AF:35:LYS:N      | 2.27                     | 0.49              |
| 6:AF:93:LYS:CG    | 6:AF:93:LYS:O      | 2.60                     | 0.49              |
| 9:AI:84:THR:HG21  | 9:AI:103:PHE:CB    | 2.42                     | 0.49              |
| 9:AI:17:ALA:CB    | 9:AI:67:VAL:HB     | 2.43                     | 0.49              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 11:AK:67:ALA:HB1  | 11:AK:100:LEU:HD22 | 1.94                     | 0.49              |
| 53:B5:215:VAL:O   | 53:B5:216:THR:CB   | 2.60                     | 0.49              |
| 53:B5:67:HIS:CD2  | 53:B5:69:LEU:HD23  | 2.47                     | 0.49              |
| 22:BA:1412:U:H2'  | 22:BA:1413:A:C8    | 2.48                     | 0.49              |
| 22:BA:2127:G:H4'  | 22:BA:2128:G:OP1   | 2.12                     | 0.49              |
| 22:BA:2409:G:H2'  | 22:BA:2410:G:O4'   | 2.12                     | 0.49              |
| 22:BA:866:A:C8    | 22:BA:914:G:C6     | 3.00                     | 0.49              |
| 25:BD:38:LYS:O    | 25:BD:46:ARG:HA    | 2.13                     | 0.49              |
| 27:BF:42:GLU:O    | 27:BF:42:GLU:HG2   | 2.13                     | 0.49              |
| 30:BI:130:GLU:HB3 | 30:BI:134:ARG:NH2  | 2.27                     | 0.49              |
| 34:BM:69:PRO:O    | 34:BM:70:ASP:CG    | 2.51                     | 0.49              |
| 35:BN:51:LEU:O    | 35:BN:52:ILE:C     | 2.49                     | 0.49              |
| 39:BR:49:ILE:CB   | 39:BR:52:PRO:C     | 2.78                     | 0.49              |
| 42:BU:37:GLU:O    | 42:BU:39:ILE:HG12  | 2.12                     | 0.49              |
| 1:CA:1048:G:P     | 57:CA:1849:HOH:O   | 2.70                     | 0.49              |
| 1:CA:1152:A:C4    | 1:CA:1153:G:C8     | 3.00                     | 0.49              |
| 1:CA:1321:U:C4    | 1:CA:1322:C:C5     | 3.00                     | 0.49              |
| 1:CA:1380:U:C5    | 7:CG:3:ARG:HA      | 2.46                     | 0.49              |
| 1:CA:246:A:C4     | 1:CA:279:A:C6      | 3.01                     | 0.49              |
| 1:CA:728:A:H2'    | 1:CA:729:A:H8      | 1.77                     | 0.49              |
| 7:CG:114:LYS:HB2  | 7:CG:118:LEU:HD12  | 1.95                     | 0.49              |
| 12:CL:61:PHE:N    | 12:CL:61:PHE:HD1   | 2.11                     | 0.49              |
| 12:CL:90:LEU:HB3  | 12:CL:93:VAL:HG21  | 1.95                     | 0.49              |
| 17:CQ:81:LYS:N    | 17:CQ:81:LYS:CD    | 2.75                     | 0.49              |
| 22:DA:1029:A:N7   | 22:DA:1030:C:C2    | 2.81                     | 0.49              |
| 22:DA:1097:U:O2   | 30:DI:9:VAL:CG1    | 2.61                     | 0.49              |
| 22:DA:1178:C:N4   | 22:DA:1180:U:N3    | 2.61                     | 0.49              |
| 22:DA:1230:A:C2   | 22:DA:1231:U:C2    | 2.99                     | 0.49              |
| 22:DA:1357:C:N4   | 22:DA:1358:G:N1    | 2.61                     | 0.49              |
| 22:DA:1403:A:C2   | 22:DA:1404:C:C2    | 3.00                     | 0.49              |
| 22:DA:1465:G:C5   | 22:DA:1466:U:C4    | 3.00                     | 0.49              |
| 22:DA:1488:C:N3   | 22:DA:1489:C:C5    | 2.81                     | 0.49              |
| 22:DA:1394:U:H4'  | 22:DA:1603:A:H4'   | 1.95                     | 0.49              |
| 22:DA:2234:G:C6   | 22:DA:2235:G:C5    | 3.01                     | 0.49              |
| 22:DA:2428:G:H5'' | 22:DA:2429:G:OP1   | 2.13                     | 0.49              |
| 22:DA:301:G:C2    | 22:DA:302:C:N3     | 2.81                     | 0.49              |
| 22:DA:804:A:H5''  | 22:DA:805:G:OP1    | 2.13                     | 0.49              |
| 24:DC:232:HIS:NE2 | 24:DC:244:PRO:HA   | 2.28                     | 0.49              |
| 31:DJ:94:ALA:O    | 31:DJ:95:ARG:C     | 2.51                     | 0.49              |
| 35:DN:28:LEU:CG   | 35:DN:28:LEU:O     | 2.61                     | 0.49              |
| 41:DT:44:LYS:O    | 41:DT:48:GLN:HG2   | 2.12                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 41:DT:28:ASN:HB3  | 41:DT:87:LEU:HB2  | 1.94                     | 0.49              |
| 45:DX:68:LEU:HD22 | 45:DX:78:TYR:CZ   | 2.47                     | 0.49              |
| 1:AA:1124:G:H3'   | 1:AA:1145:A:N6    | 2.28                     | 0.49              |
| 1:AA:1160:G:O2'   | 1:AA:1161:C:O5'   | 2.27                     | 0.49              |
| 1:AA:1452:C:O4'   | 1:AA:1453:G:N2    | 2.46                     | 0.49              |
| 1:AA:257:G:C2     | 1:AA:258:G:C5     | 3.00                     | 0.49              |
| 1:AA:568:G:C2     | 1:AA:569:C:C6     | 3.01                     | 0.49              |
| 1:AA:631:C:H5'    | 1:AA:632:U:O5'    | 2.13                     | 0.49              |
| 2:AB:96:TRP:HZ2   | 2:AB:101:LEU:CD2  | 2.25                     | 0.49              |
| 3:AC:59:ARG:HA    | 3:AC:63:SER:O     | 2.12                     | 0.49              |
| 12:AL:23:ALA:O    | 12:AL:24:LEU:O    | 2.30                     | 0.49              |
| 17:AQ:15:ASP:OD1  | 17:AQ:16:LYS:N    | 2.45                     | 0.49              |
| 21:AU:37:PHE:HB3  | 21:AU:41:PRO:HG3  | 1.94                     | 0.49              |
| 22:BA:1074:G:H2'  | 22:BA:1075:C:C6   | 2.47                     | 0.49              |
| 22:BA:1583:A:HO2' | 22:BA:1584:U:P    | 2.36                     | 0.49              |
| 22:BA:197:A:C6    | 22:BA:198:C:C2    | 3.01                     | 0.49              |
| 22:BA:2307:G:H4'  | 22:BA:2308:G:O5'  | 2.13                     | 0.49              |
| 22:BA:2517:C:C5   | 22:BA:2542:A:C5   | 3.00                     | 0.49              |
| 22:BA:26:G:C6     | 22:BA:27:G:N1     | 2.81                     | 0.49              |
| 22:BA:2751:G:C4   | 28:BG:3:ARG:HD2   | 2.47                     | 0.49              |
| 22:BA:574:A:H4'   | 22:BA:575:A:O5'   | 2.13                     | 0.49              |
| 22:BA:65:U:H2'    | 22:BA:66:C:C6     | 2.47                     | 0.49              |
| 22:BA:998:C:P     | 38:BQ:92:ARG:HH21 | 2.36                     | 0.49              |
| 42:BU:42:VAL:O    | 42:BU:60:GLU:HA   | 2.13                     | 0.49              |
| 1:CA:1296:C:H4'   | 1:CA:1302:C:C4    | 2.47                     | 0.49              |
| 1:CA:198:G:O2'    | 1:CA:199:A:H5'    | 2.12                     | 0.49              |
| 1:CA:216:U:H2'    | 1:CA:217:C:C6     | 2.47                     | 0.49              |
| 1:CA:718:A:H5''   | 11:CK:119:ASN:ND2 | 2.28                     | 0.49              |
| 1:CA:881:G:C6     | 1:CA:882:C:C4     | 3.01                     | 0.49              |
| 3:CC:130:PHE:CE1  | 3:CC:157:LEU:HB3  | 2.48                     | 0.49              |
| 14:CN:87:ALA:HB1  | 14:CN:92:GLU:HB2  | 1.95                     | 0.49              |
| 21:CU:37:PHE:CD2  | 21:CU:41:PRO:HG3  | 2.48                     | 0.49              |
| 22:DA:1096:A:C8   | 22:DA:1096:A:OP2  | 2.65                     | 0.49              |
| 22:DA:1287:A:C2'  | 22:DA:1288:G:H5'  | 2.42                     | 0.49              |
| 22:DA:1357:C:H2'  | 22:DA:1358:G:C5'  | 2.42                     | 0.49              |
| 22:DA:1361:G:C5   | 22:DA:1371:G:N2   | 2.80                     | 0.49              |
| 22:DA:1439:A:N7   | 22:DA:1552:A:H2   | 2.10                     | 0.49              |
| 22:DA:1819:A:H4'  | 22:DA:1820:U:H5'' | 1.93                     | 0.49              |
| 22:DA:2098:U:H2'  | 22:DA:2099:U:C6   | 2.48                     | 0.49              |
| 22:DA:2497:A:N3   | 22:DA:2498:C:N4   | 2.61                     | 0.49              |
| 22:DA:2507:C:N4   | 22:DA:2508:G:C6   | 2.81                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:DA:2693:G:N2   | 22:DA:2717:C:C2   | 2.81                     | 0.49              |
| 22:DA:301:G:C2    | 22:DA:302:C:C2    | 3.01                     | 0.49              |
| 22:DA:79:C:C2'    | 22:DA:346:A:N3    | 2.76                     | 0.49              |
| 22:DA:581:C:OP2   | 38:DQ:33:ARG:NE   | 2.45                     | 0.49              |
| 22:DA:631:A:N3    | 22:DA:2415:G:O2'  | 2.45                     | 0.49              |
| 22:DA:749:A:C6    | 22:DA:1618:A:C2   | 3.01                     | 0.49              |
| 22:DA:801:G:C8    | 26:DE:49:ARG:HG3  | 2.48                     | 0.49              |
| 22:DA:846:U:O2'   | 22:DA:847:U:P     | 2.70                     | 0.49              |
| 22:DA:969:G:H2'   | 22:DA:970:U:C6    | 2.48                     | 0.49              |
| 23:DB:30:C:OP1    | 36:DO:3:LYS:NZ    | 2.45                     | 0.49              |
| 29:DH:72:ILE:O    | 29:DH:141:LYS:O   | 2.30                     | 0.49              |
| 30:DI:28:LEU:HD13 | 30:DI:38:PHE:CE2  | 2.48                     | 0.49              |
| 34:DM:69:PRO:O    | 34:DM:70:ASP:HB3  | 2.11                     | 0.49              |
| 40:DS:61:ASN:O    | 40:DS:62:ASP:HB3  | 2.13                     | 0.49              |
| 42:DU:86:ARG:NH2  | 42:DU:95:PHE:HB3  | 2.28                     | 0.49              |
| 45:DX:71:LEU:HA   | 45:DX:74:ARG:HG2  | 1.94                     | 0.49              |
| 1:AA:976:G:OP2    | 1:AA:1358:U:O2'   | 2.30                     | 0.49              |
| 1:AA:771:G:C2'    | 1:AA:772:U:H5'    | 2.43                     | 0.49              |
| 1:AA:782:A:C8     | 1:AA:783:C:C5     | 3.01                     | 0.49              |
| 1:AA:404:G:N7     | 4:AD:2:ALA:CB     | 2.76                     | 0.49              |
| 5:AE:13:GLU:HB3   | 5:AE:39:VAL:HG12  | 1.94                     | 0.49              |
| 6:AF:54:LEU:O     | 6:AF:54:LEU:HD13  | 2.12                     | 0.49              |
| 7:AG:115:SER:OG   | 7:AG:118:LEU:HG   | 2.12                     | 0.49              |
| 12:AL:44:LYS:CB   | 12:AL:45:PRO:HD3  | 2.43                     | 0.49              |
| 17:AQ:17:MET:HG2  | 17:AQ:20:SER:HB3  | 1.95                     | 0.49              |
| 17:AQ:81:LYS:O    | 17:AQ:82:ALA:C    | 2.50                     | 0.49              |
| 53:B5:24:ASP:HB3  | 53:B5:185:LYS:O   | 2.13                     | 0.49              |
| 22:BA:1914:C:C2   | 22:BA:1915:U:C6   | 3.00                     | 0.49              |
| 22:BA:2356:U:O3'  | 44:BW:20:ARG:HD3  | 2.13                     | 0.49              |
| 22:BA:477:A:H2'   | 22:BA:478:A:C8    | 2.47                     | 0.49              |
| 22:BA:876:C:N3    | 22:BA:901:C:N4    | 2.61                     | 0.49              |
| 22:BA:88:G:C6     | 22:BA:89:A:N7     | 2.80                     | 0.49              |
| 25:BD:62:LYS:N    | 25:BD:63:PRO:CD   | 2.75                     | 0.49              |
| 30:BI:24:VAL:CG2  | 30:BI:28:LEU:HD23 | 2.43                     | 0.49              |
| 33:BL:109:LYS:HG2 | 33:BL:126:ARG:CB  | 2.43                     | 0.49              |
| 34:BM:77:PRO:HD2  | 34:BM:80:VAL:HG21 | 1.94                     | 0.49              |
| 1:CA:1337:G:H5''  | 1:CA:1338:G:OP1   | 2.13                     | 0.49              |
| 1:CA:161:A:H2'    | 1:CA:162:A:C8     | 2.48                     | 0.49              |
| 1:CA:16:A:C2'     | 1:CA:17:U:H5'     | 2.43                     | 0.49              |
| 1:CA:630:A:H2'    | 1:CA:631:C:O4'    | 2.13                     | 0.49              |
| 2:CB:67:ILE:HG22  | 2:CB:68:LEU:N     | 2.28                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:CD:146:ARG:O    | 4:CD:148:LYS:O    | 2.30                     | 0.49              |
| 12:CL:42:PRO:HD3  | 12:CL:48:ALA:O    | 2.13                     | 0.49              |
| 12:CL:94:ARG:O    | 12:CL:95:TYR:CD1  | 2.66                     | 0.49              |
| 14:CN:46:LEU:O    | 14:CN:46:LEU:HG   | 2.13                     | 0.49              |
| 22:DA:123:G:N2    | 22:DA:129:C:C2    | 2.80                     | 0.49              |
| 22:DA:1267:U:N3   | 22:DA:2013:A:N7   | 2.60                     | 0.49              |
| 22:DA:1312:U:H3'  | 57:DA:3387:HOH:O  | 2.13                     | 0.49              |
| 22:DA:1863:G:H2'  | 22:DA:1864:U:O4'  | 2.12                     | 0.49              |
| 22:DA:192:C:O2'   | 22:DA:802:A:N3    | 2.45                     | 0.49              |
| 22:DA:2111:U:O4   | 22:DA:2147:A:C2   | 2.66                     | 0.49              |
| 22:DA:308:G:C8    | 22:DA:501:A:H1'   | 2.48                     | 0.49              |
| 22:DA:680:C:H2'   | 22:DA:681:G:C8    | 2.48                     | 0.49              |
| 22:DA:846:U:HO2'  | 22:DA:847:U:P     | 2.36                     | 0.49              |
| 22:DA:858:G:N2    | 22:DA:919:U:O4    | 2.43                     | 0.49              |
| 22:DA:1566:A:N3   | 24:DC:213:TRP:CG  | 2.80                     | 0.49              |
| 24:DC:80:ARG:NH1  | 24:DC:82:GLU:OE2  | 2.46                     | 0.49              |
| 26:DE:18:THR:HG22 | 26:DE:19:PHE:CD2  | 2.47                     | 0.49              |
| 22:DA:443:A:C8    | 26:DE:40:ARG:CG   | 2.96                     | 0.49              |
| 32:DK:17:ARG:HG2  | 32:DK:47:ILE:CG2  | 2.43                     | 0.49              |
| 32:DK:30:ARG:NH2  | 32:DK:37:ASP:OD1  | 2.46                     | 0.49              |
| 40:DS:39:THR:O    | 40:DS:41:LYS:N    | 2.46                     | 0.49              |
| 41:DT:30:ILE:HD13 | 41:DT:32:LEU:HG   | 1.93                     | 0.49              |
| 1:AA:202:G:N2     | 1:AA:216:U:O2     | 2.46                     | 0.49              |
| 1:AA:478:A:H2'    | 1:AA:479:U:C5'    | 2.42                     | 0.49              |
| 1:AA:548:G:O2'    | 1:AA:549:C:H5'    | 2.13                     | 0.49              |
| 1:AA:581:G:C5     | 1:AA:758:C:C5     | 3.01                     | 0.49              |
| 1:AA:649:A:H2'    | 1:AA:650:G:O4'    | 2.13                     | 0.49              |
| 3:AC:23:PHE:CD2   | 3:AC:24:ALA:N     | 2.81                     | 0.49              |
| 4:AD:125:VAL:O    | 4:AD:126:ASN:C    | 2.52                     | 0.49              |
| 9:AI:30:ILE:HD11  | 9:AI:38:TYR:HB3   | 1.94                     | 0.49              |
| 13:AM:2:ALA:O     | 13:AM:9:ILE:HG23  | 2.13                     | 0.49              |
| 16:AP:70:ARG:O    | 16:AP:70:ARG:CG   | 2.61                     | 0.49              |
| 17:AQ:47:HIS:HB2  | 17:AQ:67:LEU:HD23 | 1.95                     | 0.49              |
| 49:B1:19:HIS:HE1  | 49:B1:21:TYR:CE2  | 2.31                     | 0.49              |
| 22:BA:996:A:N6    | 22:BA:1160:G:C6   | 2.81                     | 0.49              |
| 22:BA:1513:U:H2'  | 22:BA:1514:G:O4'  | 2.13                     | 0.49              |
| 22:BA:1686:C:H2'  | 22:BA:1687:G:O4'  | 2.13                     | 0.49              |
| 22:BA:1915:U:H2'  | 22:BA:1916:A:H5'  | 1.94                     | 0.49              |
| 22:BA:205:G:O2'   | 22:BA:206:U:P     | 2.71                     | 0.49              |
| 22:BA:2480:C:H2'  | 22:BA:2481:G:H5'  | 1.95                     | 0.49              |
| 22:BA:2780:G:OP2  | 31:BJ:120:ARG:HD3 | 2.13                     | 0.49              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 22:BA:319:G:C5     | 22:BA:333:G:C2    | 3.01                     | 0.49              |
| 22:BA:475:C:N4     | 22:BA:476:G:C6    | 2.80                     | 0.49              |
| 22:BA:545:U:H2'    | 22:BA:546:U:O3'   | 2.13                     | 0.49              |
| 22:BA:861:A:C2     | 22:BA:917:A:C4    | 3.01                     | 0.49              |
| 23:BB:42:C:OP1     | 27:BF:64:LYS:HE2  | 2.13                     | 0.49              |
| 24:BC:167:ARG:O    | 24:BC:168:ASP:CB  | 2.60                     | 0.49              |
| 25:BD:103:ASP:O    | 25:BD:104:VAL:CG2 | 2.61                     | 0.49              |
| 25:BD:129:THR:HG23 | 25:BD:130:GLN:O   | 2.12                     | 0.49              |
| 31:BJ:64:VAL:CG1   | 31:BJ:68:LYS:HB2  | 2.43                     | 0.49              |
| 34:BM:132:THR:CG2  | 34:BM:133:LYS:N   | 2.76                     | 0.49              |
| 36:BO:100:HIS:O    | 36:BO:104:GLN:HB2 | 2.13                     | 0.49              |
| 1:CA:1074:G:H4'    | 2:CB:102:THR:O    | 2.12                     | 0.49              |
| 1:CA:1082:A:C6     | 1:CA:1083:U:N3    | 2.81                     | 0.49              |
| 1:CA:1361:G:C4     | 1:CA:1362:A:N7    | 2.81                     | 0.49              |
| 1:CA:157:U:O2'     | 1:CA:158:G:H5'    | 2.12                     | 0.49              |
| 1:CA:215:C:H2'     | 1:CA:216:U:O4'    | 2.13                     | 0.49              |
| 1:CA:620:C:H2'     | 1:CA:621:A:O4'    | 2.13                     | 0.49              |
| 1:CA:757:U:OP1     | 1:CA:822:U:O2'    | 2.17                     | 0.49              |
| 1:CA:786:G:C2      | 1:CA:787:A:H1'    | 2.47                     | 0.49              |
| 1:CA:834:U:N3      | 1:CA:835:U:C4     | 2.81                     | 0.49              |
| 3:CC:81:GLY:O      | 3:CC:83:ASP:N     | 2.46                     | 0.49              |
| 4:CD:168:PRO:CB    | 4:CD:171:LEU:CD1  | 2.91                     | 0.49              |
| 5:CE:13:GLU:HB2    | 5:CE:39:VAL:HG12  | 1.95                     | 0.49              |
| 8:CH:106:THR:HG21  | 8:CH:121:LEU:HD13 | 1.95                     | 0.49              |
| 21:CU:37:PHE:CD1   | 21:CU:40:LYS:HE3  | 2.47                     | 0.49              |
| 21:CU:40:LYS:N     | 21:CU:41:PRO:CD   | 2.76                     | 0.49              |
| 22:DA:1049:C:H2'   | 22:DA:1050:A:H5'  | 1.95                     | 0.49              |
| 22:DA:1317:G:N7    | 22:DA:1318:U:C4   | 2.81                     | 0.49              |
| 22:DA:1319:C:H2'   | 22:DA:1320:C:H5'  | 1.94                     | 0.49              |
| 22:DA:1378:A:N3    | 22:DA:1379:U:H2'  | 2.28                     | 0.49              |
| 22:DA:1574:C:N4    | 57:DA:3620:HOH:O  | 2.46                     | 0.49              |
| 22:DA:1826:G:C4    | 22:DA:1827:U:C5   | 3.01                     | 0.49              |
| 22:DA:1958:C:P     | 57:DA:3730:HOH:O  | 2.71                     | 0.49              |
| 22:DA:2024:G:N2    | 22:DA:2040:G:H1'  | 2.28                     | 0.49              |
| 22:DA:204:A:H5'    | 22:DA:206:U:O4'   | 2.12                     | 0.49              |
| 22:DA:2734:A:C8    | 22:DA:2735:G:C8   | 3.01                     | 0.49              |
| 22:DA:2791:G:O6    | 22:DA:2805:C:N3   | 2.45                     | 0.49              |
| 22:DA:2873:A:H4'   | 57:DA:3802:HOH:O  | 2.11                     | 0.49              |
| 22:DA:362:A:N7     | 22:DA:363:G:N7    | 2.61                     | 0.49              |
| 22:DA:38:A:H5'     | 26:DE:45:ALA:HB3  | 1.93                     | 0.49              |
| 22:DA:475:C:N3     | 22:DA:481:G:C6    | 2.81                     | 0.49              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:DA:7:G:H4'     | 31:DJ:15:TRP:CH2  | 2.47                     | 0.49              |
| 24:DC:148:PRO:HD3 | 24:DC:185:GLU:OE2 | 2.13                     | 0.49              |
| 25:DD:2:ILE:HG23  | 25:DD:88:GLU:OE2  | 2.12                     | 0.49              |
| 36:DO:76:LYS:O    | 36:DO:79:ALA:HB3  | 2.12                     | 0.49              |
| 41:DT:61:LEU:C    | 41:DT:61:LEU:HD12 | 2.32                     | 0.49              |
| 41:DT:77:ARG:O    | 41:DT:78:SER:CB   | 2.60                     | 0.49              |
| 43:DV:75:GLN:HB3  | 43:DV:90:ASP:O    | 2.12                     | 0.49              |
| 1:AA:1029:U:O2'   | 1:AA:1032:G:O6    | 2.31                     | 0.48              |
| 1:AA:1426:G:H2'   | 1:AA:1427:C:O4'   | 2.13                     | 0.48              |
| 1:AA:452:A:H2'    | 1:AA:453:G:H5'    | 1.95                     | 0.48              |
| 1:AA:723:U:H4'    | 1:AA:723:U:OP2    | 2.11                     | 0.48              |
| 1:AA:914:A:C4     | 1:AA:915:A:C8     | 3.01                     | 0.48              |
| 2:AB:72:THR:O     | 2:AB:73:LYS:CB    | 2.60                     | 0.48              |
| 8:AH:78:VAL:HG11  | 8:AH:125:ILE:CD1  | 2.43                     | 0.48              |
| 12:AL:85:GLY:O    | 12:AL:96:HIS:ND1  | 2.45                     | 0.48              |
| 13:AM:11:ASP:CG   | 13:AM:12:HIS:N    | 2.64                     | 0.48              |
| 15:AO:81:LEU:CD1  | 15:AO:85:LEU:CD2  | 2.91                     | 0.48              |
| 22:BA:1624:U:C2   | 22:BA:1625:C:C6   | 3.01                     | 0.48              |
| 22:BA:2488:G:O2'  | 22:BA:2489:U:H5'  | 2.12                     | 0.48              |
| 22:BA:2832:U:C2   | 22:BA:2834:G:C2   | 3.01                     | 0.48              |
| 22:BA:753:A:H2'   | 22:BA:754:U:H6    | 1.78                     | 0.48              |
| 24:BC:235:GLY:HA3 | 24:BC:239:ASN:HB2 | 1.94                     | 0.48              |
| 29:BH:139:PHE:O   | 29:BH:140:ALA:HB2 | 2.13                     | 0.48              |
| 22:BA:580:U:O3'   | 38:BQ:31:VAL:CG1  | 2.61                     | 0.48              |
| 41:BT:19:LYS:NZ   | 41:BT:84:TYR:OH   | 2.46                     | 0.48              |
| 1:CA:1211:U:O2'   | 1:CA:1212:U:P     | 2.70                     | 0.48              |
| 1:CA:1240:U:OP2   | 7:CG:116:MET:HB3  | 2.12                     | 0.48              |
| 1:CA:9:G:OP2      | 5:CE:126:LYS:NZ   | 2.44                     | 0.48              |
| 3:CC:83:ASP:O     | 3:CC:84:VAL:C     | 2.52                     | 0.48              |
| 5:CE:35:ALA:O     | 5:CE:50:TYR:O     | 2.31                     | 0.48              |
| 5:CE:50:TYR:O     | 5:CE:51:GLY:O     | 2.31                     | 0.48              |
| 7:CG:42:ILE:HG21  | 7:CG:116:MET:HG3  | 1.95                     | 0.48              |
| 9:CI:13:LYS:O     | 9:CI:14:SER:HB3   | 2.12                     | 0.48              |
| 13:CM:29:ARG:NH1  | 13:CM:59:GLU:O    | 2.46                     | 0.48              |
| 14:CN:10:GLU:O    | 14:CN:11:VAL:C    | 2.50                     | 0.48              |
| 50:D2:18:PHE:O    | 50:D2:19:ARG:C    | 2.51                     | 0.48              |
| 22:DA:1338:G:H5'' | 41:DT:17:SER:HB2  | 1.94                     | 0.48              |
| 22:DA:1352:U:H5   | 22:DA:1377:G:C5   | 2.31                     | 0.48              |
| 22:DA:1400:U:H2'  | 22:DA:1401:G:O4'  | 2.12                     | 0.48              |
| 22:DA:1792:G:C5   | 22:DA:1793:C:C5   | 3.01                     | 0.48              |
| 22:DA:1916:A:H2'  | 22:DA:1917:U:O4'  | 2.13                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:DA:2272:U:H5'' | 22:DA:2273:A:OP1  | 2.12                     | 0.48              |
| 22:DA:230:G:C2    | 22:DA:231:A:N7    | 2.81                     | 0.48              |
| 22:DA:2446:G:C6   | 22:DA:2501:C:H2'  | 2.48                     | 0.48              |
| 22:DA:245:G:O6    | 51:D3:8:ARG:HD2   | 2.12                     | 0.48              |
| 22:DA:2512:C:H2'  | 22:DA:2513:A:O4'  | 2.12                     | 0.48              |
| 22:DA:279:A:N6    | 22:DA:361:G:C2'   | 2.75                     | 0.48              |
| 22:DA:323:C:O4'   | 22:DA:323:C:O2    | 2.31                     | 0.48              |
| 22:DA:649:G:H2'   | 22:DA:650:C:C6    | 2.48                     | 0.48              |
| 22:DA:711:G:C2    | 22:DA:721:A:N3    | 2.81                     | 0.48              |
| 22:DA:920:A:C6    | 22:DA:921:C:C4    | 3.01                     | 0.48              |
| 24:DC:62:TYR:CD1  | 24:DC:63:ARG:N    | 2.80                     | 0.48              |
| 25:DD:186:LEU:CD1 | 37:DP:8:LEU:HD12  | 2.43                     | 0.48              |
| 31:DJ:84:ILE:CG1  | 31:DJ:84:ILE:O    | 2.61                     | 0.48              |
| 34:DM:1:MET:HE3   | 34:DM:43:ALA:HB3  | 1.95                     | 0.48              |
| 22:DA:310:A:H5''  | 42:DU:15:THR:HB   | 1.95                     | 0.48              |
| 42:DU:96:PHE:CZ   | 42:DU:103:ILE:CG1 | 2.96                     | 0.48              |
| 1:AA:1107:C:C4    | 1:AA:1108:G:C8    | 3.01                     | 0.48              |
| 1:AA:1195:C:H5''  | 1:AA:1196:A:OP2   | 2.13                     | 0.48              |
| 1:AA:1349:A:C2    | 1:AA:1374:A:C5    | 3.01                     | 0.48              |
| 1:AA:233:C:H2'    | 1:AA:234:C:C6     | 2.48                     | 0.48              |
| 1:AA:747:A:C5'    | 1:AA:748:G:OP2    | 2.61                     | 0.48              |
| 2:AB:133:GLU:OE2  | 2:AB:137:ARG:NH1  | 2.47                     | 0.48              |
| 5:AE:16:ILE:CG2   | 5:AE:110:ALA:HA   | 2.43                     | 0.48              |
| 5:AE:60:ILE:HD13  | 5:AE:61:GLN:N     | 2.28                     | 0.48              |
| 6:AF:42:TRP:HB2   | 6:AF:59:TYR:HB2   | 1.95                     | 0.48              |
| 11:AK:112:ASP:OD1 | 21:AU:24:GLU:OE2  | 2.31                     | 0.48              |
| 12:AL:35:THR:HG21 | 12:AL:54:ARG:NH2  | 2.28                     | 0.48              |
| 12:AL:43:LYS:O    | 12:AL:44:LYS:C    | 2.51                     | 0.48              |
| 18:AR:28:THR:O    | 18:AR:31:ASN:ND2  | 2.45                     | 0.48              |
| 19:AS:58:VAL:CG1  | 19:AS:75:ALA:HB1  | 2.43                     | 0.48              |
| 21:AU:12:PHE:CD1  | 21:AU:16:LEU:CD1  | 2.96                     | 0.48              |
| 22:BA:1176:U:H2'  | 22:BA:1177:G:C4   | 2.49                     | 0.48              |
| 22:BA:150:U:H2'   | 22:BA:151:C:C6    | 2.48                     | 0.48              |
| 22:BA:2188:U:C4   | 22:BA:2189:U:C4   | 3.02                     | 0.48              |
| 22:BA:2250:G:O5'  | 22:BA:2250:G:H8   | 1.96                     | 0.48              |
| 22:BA:2271:G:H2'  | 22:BA:2272:U:O4'  | 2.13                     | 0.48              |
| 22:BA:2371:G:C2   | 22:BA:2372:U:C6   | 3.01                     | 0.48              |
| 22:BA:2377:A:O2'  | 22:BA:2378:A:H5'  | 2.14                     | 0.48              |
| 22:BA:273:G:N2    | 22:BA:365:U:O2    | 2.46                     | 0.48              |
| 22:BA:2861:U:C2   | 22:BA:2862:G:C8   | 3.01                     | 0.48              |
| 22:BA:31:C:O3'    | 22:BA:1238:G:H5'' | 2.13                     | 0.48              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 26:BE:42:GLY:HA3  | 26:BE:90:GLN:O     | 2.13                     | 0.48              |
| 26:BE:77:ILE:O    | 26:BE:77:ILE:CG1   | 2.61                     | 0.48              |
| 1:CA:734:G:C4     | 1:CA:735:C:C6      | 3.01                     | 0.48              |
| 1:CA:8:A:N6       | 4:CD:54:GLN:OE1    | 2.46                     | 0.48              |
| 2:CB:71:GLY:CA    | 2:CB:164:ILE:CG2   | 2.91                     | 0.48              |
| 5:CE:149:SER:OG   | 5:CE:152:MET:HB2   | 2.13                     | 0.48              |
| 5:CE:33:PHE:O     | 5:CE:52:LYS:HB2    | 2.13                     | 0.48              |
| 5:CE:96:MET:CE    | 5:CE:111:MET:CE    | 2.90                     | 0.48              |
| 6:CF:43:GLY:HA2   | 6:CF:58:HIS:CD2    | 2.48                     | 0.48              |
| 6:CF:66:ALA:HB3   | 6:CF:71:ILE:HD11   | 1.93                     | 0.48              |
| 10:CJ:73:LEU:CD2  | 10:CJ:75:ASP:HB2   | 2.42                     | 0.48              |
| 10:CJ:82:LYS:O    | 10:CJ:86:ALA:HB3   | 2.13                     | 0.48              |
| 14:CN:62:ASN:HB3  | 14:CN:73:PHE:CD1   | 2.48                     | 0.48              |
| 51:D3:16:LYS:HE3  | 51:D3:20:GLY:O     | 2.13                     | 0.48              |
| 22:DA:1577:C:H2'  | 22:DA:1578:U:O4'   | 2.13                     | 0.48              |
| 22:DA:1731:G:N1   | 22:DA:1733:G:C4    | 2.81                     | 0.48              |
| 22:DA:1751:U:H2'  | 22:DA:1752:C:C6    | 2.48                     | 0.48              |
| 22:DA:1856:U:C4   | 22:DA:1857:G:C6    | 3.01                     | 0.48              |
| 22:DA:1981:A:H5'' | 22:DA:1982:U:OP2   | 2.13                     | 0.48              |
| 22:DA:2025:C:H2'  | 22:DA:2026:U:C6    | 2.48                     | 0.48              |
| 22:DA:2174:C:H2'  | 22:DA:2175:C:O4'   | 2.12                     | 0.48              |
| 22:DA:2543:G:N3   | 22:DA:2765:A:H2'   | 2.28                     | 0.48              |
| 37:DP:106:LYS:O   | 37:DP:109:ARG:HD2  | 2.14                     | 0.48              |
| 37:DP:99:TYR:CE2  | 37:DP:100:LEU:HD21 | 2.48                     | 0.48              |
| 44:DW:46:HIS:CD2  | 44:DW:77:ARG:HD3   | 2.48                     | 0.48              |
| 47:DZ:10:THR:HG23 | 47:DZ:54:MET:C     | 2.32                     | 0.48              |
| 1:AA:1149:C:O2'   | 1:AA:1150:A:H5'    | 2.14                     | 0.48              |
| 1:AA:926:G:C6     | 1:AA:1505:G:C5     | 3.01                     | 0.48              |
| 1:AA:43:C:H2'     | 1:AA:44:A:O4'      | 2.13                     | 0.48              |
| 1:AA:781:A:C4     | 1:AA:802:A:C2      | 3.01                     | 0.48              |
| 2:AB:120:GLN:O    | 2:AB:120:GLN:HG2   | 2.13                     | 0.48              |
| 2:AB:49:MET:O     | 2:AB:51:ASN:O      | 2.31                     | 0.48              |
| 5:AE:69:ARG:O     | 5:AE:70:ASN:C      | 2.50                     | 0.48              |
| 5:AE:74:VAL:HG23  | 5:AE:76:LEU:CD1    | 2.43                     | 0.48              |
| 1:AA:1349:A:OP1   | 9:AI:120:LYS:O     | 2.31                     | 0.48              |
| 9:AI:80:ARG:HD2   | 9:AI:80:ARG:O      | 2.13                     | 0.48              |
| 10:AJ:59:LYS:HD2  | 10:AJ:59:LYS:N     | 2.27                     | 0.48              |
| 22:BA:1528:A:H2'  | 22:BA:1529:G:O4'   | 2.13                     | 0.48              |
| 22:BA:1832:C:N4   | 22:BA:1833:C:C4    | 2.80                     | 0.48              |
| 22:BA:2310:C:H2'  | 22:BA:2311:A:C5'   | 2.42                     | 0.48              |
| 22:BA:2435:A:C2'  | 22:BA:2436:G:O5'   | 2.61                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 26:BE:31:VAL:HG21  | 26:BE:104:ALA:HB2  | 1.95                     | 0.48              |
| 27:BF:122:PHE:HB3  | 27:BF:163:ASP:CG   | 2.33                     | 0.48              |
| 30:BI:97:LYS:HG2   | 30:BI:139:VAL:HG22 | 1.94                     | 0.48              |
| 32:BK:35:VAL:CG1   | 32:BK:106:GLU:HG2  | 2.44                     | 0.48              |
| 32:BK:86:LEU:N     | 32:BK:86:LEU:HD23  | 2.28                     | 0.48              |
| 35:BN:70:THR:OG1   | 35:BN:71:ARG:N     | 2.46                     | 0.48              |
| 39:BR:14:VAL:HG13  | 39:BR:98:ILE:HG13  | 1.95                     | 0.48              |
| 39:BR:25:LEU:O     | 39:BR:94:THR:HG21  | 2.13                     | 0.48              |
| 1:CA:1019:A:H2'    | 1:CA:1020:G:O4'    | 2.14                     | 0.48              |
| 1:CA:1181:G:O2'    | 1:CA:1182:G:C5     | 2.64                     | 0.48              |
| 1:CA:158:G:C5      | 1:CA:164:G:C6      | 3.01                     | 0.48              |
| 1:CA:3:A:O2'       | 1:CA:612:C:O2'     | 2.26                     | 0.48              |
| 29:BH:91:PHE:O     | 1:CA:55:A:N1       | 2.47                     | 0.48              |
| 1:CA:728:A:C2      | 1:CA:729:A:C5      | 3.01                     | 0.48              |
| 2:CB:20:THR:OG1    | 2:CB:21:ARG:N      | 2.46                     | 0.48              |
| 9:CI:116:VAL:HG23  | 10:CJ:62:ARG:HD3   | 1.96                     | 0.48              |
| 12:CL:21:VAL:N     | 12:CL:22:PRO:CD    | 2.76                     | 0.48              |
| 22:DA:1153:C:H2'   | 22:DA:1154:G:O4'   | 2.14                     | 0.48              |
| 22:DA:1211:C:H3'   | 22:DA:1212:G:H5'   | 1.94                     | 0.48              |
| 22:DA:135:U:H2'    | 22:DA:136:G:C8     | 2.48                     | 0.48              |
| 22:DA:1524:G:C2    | 22:DA:1525:A:C8    | 3.01                     | 0.48              |
| 22:DA:158:U:O2     | 22:DA:169:G:C2     | 2.66                     | 0.48              |
| 22:DA:169:G:C2     | 22:DA:170:U:C6     | 3.01                     | 0.48              |
| 22:DA:2032:G:H1'   | 25:DD:150:GLN:HE22 | 1.76                     | 0.48              |
| 22:DA:2056:G:C6    | 22:DA:2057:G:N7    | 2.82                     | 0.48              |
| 22:DA:2146:C:H4'   | 22:DA:2147:A:C8    | 2.47                     | 0.48              |
| 22:DA:2321:U:H5'   | 22:DA:2322:A:OP2   | 2.13                     | 0.48              |
| 22:DA:410:G:C2     | 22:DA:2407:A:C5    | 3.01                     | 0.48              |
| 22:DA:371:A:N6     | 22:DA:402:A:OP2    | 2.46                     | 0.48              |
| 22:DA:441:U:O2'    | 26:DE:41:GLN:OE1   | 2.27                     | 0.48              |
| 22:DA:78:U:OP2     | 46:DY:2:LYS:HD2    | 2.12                     | 0.48              |
| 24:DC:162:VAL:HG12 | 24:DC:163:GLN:N    | 2.27                     | 0.48              |
| 22:DA:1791:A:O3'   | 24:DC:205:LEU:HB2  | 2.13                     | 0.48              |
| 29:DH:127:GLU:HG3  | 29:DH:144:VAL:O    | 2.13                     | 0.48              |
| 29:DH:21:VAL:CG2   | 29:DH:22:LYS:N     | 2.76                     | 0.48              |
| 30:DI:20:PRO:HB2   | 30:DI:23:PRO:HD2   | 1.95                     | 0.48              |
| 31:DJ:71:ASP:O     | 31:DJ:73:VAL:HG23  | 2.14                     | 0.48              |
| 33:DL:2:ARG:N      | 33:DL:2:ARG:HD3    | 2.29                     | 0.48              |
| 38:DQ:78:LYS:HE2   | 38:DQ:117:LEU:HD21 | 1.95                     | 0.48              |
| 39:DR:49:ILE:HG22  | 39:DR:53:PHE:C     | 2.33                     | 0.48              |
| 42:DU:10:GLU:HG2   | 42:DU:11:VAL:N     | 2.28                     | 0.48              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 42:DU:13:VAL:HG21 | 42:DU:39:ILE:HG23  | 1.93                     | 0.48              |
| 44:DW:34:GLY:N    | 44:DW:61:ALA:O     | 2.38                     | 0.48              |
| 1:AA:1142:G:H2'   | 1:AA:1143:G:O4'    | 2.13                     | 0.48              |
| 1:AA:292:G:N7     | 1:AA:293:G:H1'     | 2.29                     | 0.48              |
| 1:AA:359:G:H2'    | 1:AA:360:G:O4'     | 2.13                     | 0.48              |
| 1:AA:69:G:O6      | 1:AA:98:A:N6       | 2.47                     | 0.48              |
| 1:AA:803:G:C6     | 1:AA:804:U:N3      | 2.82                     | 0.48              |
| 1:AA:882:C:O2'    | 1:AA:883:C:H5'     | 2.12                     | 0.48              |
| 1:AA:903:G:C5     | 1:AA:904:U:C5      | 3.01                     | 0.48              |
| 1:AA:942:G:H2'    | 1:AA:942:G:N3      | 2.27                     | 0.48              |
| 2:AB:82:ASP:C     | 2:AB:84:ALA:N      | 2.64                     | 0.48              |
| 7:AG:139:GLU:HA   | 7:AG:139:GLU:OE1   | 2.13                     | 0.48              |
| 16:AP:19:VAL:HG13 | 16:AP:37:GLY:C     | 2.34                     | 0.48              |
| 19:AS:45:ILE:HG23 | 19:AS:63:THR:HA    | 1.94                     | 0.48              |
| 51:B3:30:ARG:O    | 51:B3:31:HIS:HB3   | 2.13                     | 0.48              |
| 22:BA:1031:G:H4'  | 52:B4:6:SER:HB2    | 1.94                     | 0.48              |
| 22:BA:1075:C:H2'  | 22:BA:1076:C:C6    | 2.48                     | 0.48              |
| 22:BA:1306:C:O2   | 22:BA:1306:C:H2'   | 2.13                     | 0.48              |
| 22:BA:1682:G:C8   | 22:BA:1757:A:C2    | 3.00                     | 0.48              |
| 22:BA:1789:A:P    | 24:BC:221:ARG:HH11 | 2.37                     | 0.48              |
| 22:BA:1839:G:H2'  | 22:BA:1840:G:O5'   | 2.13                     | 0.48              |
| 22:BA:2026:U:H2'  | 22:BA:2027:G:O4'   | 2.12                     | 0.48              |
| 22:BA:2298:A:C6   | 22:BA:2321:U:O4    | 2.66                     | 0.48              |
| 22:BA:2339:C:H2'  | 22:BA:2340:A:C8    | 2.48                     | 0.48              |
| 22:BA:2502:G:H5'  | 22:BA:2503:A:H5''  | 1.94                     | 0.48              |
| 22:BA:271:G:C4    | 22:BA:367:G:N2     | 2.82                     | 0.48              |
| 22:BA:660:C:H2'   | 22:BA:661:A:C8     | 2.48                     | 0.48              |
| 24:BC:222:GLY:HA3 | 24:BC:230:HIS:CE1  | 2.48                     | 0.48              |
| 27:BF:102:ARG:HD2 | 27:BF:140:GLU:OE2  | 2.14                     | 0.48              |
| 29:BH:121:VAL:H   | 29:BH:122:LEU:HB2  | 1.77                     | 0.48              |
| 42:BU:4:LYS:O     | 42:BU:5:ILE:HD12   | 2.13                     | 0.48              |
| 1:CA:1513:A:H2'   | 1:CA:1514:G:H8     | 1.78                     | 0.48              |
| 1:CA:577:G:C2     | 1:CA:578:C:C6      | 3.02                     | 0.48              |
| 1:CA:862:C:C4     | 1:CA:863:U:C5      | 3.01                     | 0.48              |
| 2:CB:186:ILE:HA   | 2:CB:200:ILE:HB    | 1.93                     | 0.48              |
| 4:CD:73:ARG:O     | 4:CD:76:TYR:N      | 2.46                     | 0.48              |
| 7:CG:30:LEU:HD11  | 7:CG:116:MET:HE2   | 1.96                     | 0.48              |
| 7:CG:146:GLU:OE1  | 7:CG:149:LYS:CE    | 2.61                     | 0.48              |
| 14:CN:54:ASP:HA   | 14:CN:59:ARG:CD    | 2.43                     | 0.48              |
| 22:DA:1215:G:H2'  | 22:DA:1216:G:O4'   | 2.14                     | 0.48              |
| 22:DA:1262:A:C6   | 22:DA:1263:U:C2    | 3.01                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:DA:12:U:O2      | 22:DA:12:U:C2'     | 2.61                     | 0.48              |
| 22:DA:1581:G:C6    | 22:DA:1582:C:C4    | 3.01                     | 0.48              |
| 22:DA:2011:U:H2'   | 22:DA:2012:G:O4'   | 2.12                     | 0.48              |
| 22:DA:2127:G:N3    | 22:DA:2162:G:N7    | 2.61                     | 0.48              |
| 22:DA:2250:G:OP1   | 22:DA:2275:C:O2'   | 2.16                     | 0.48              |
| 22:DA:2327:A:H2'   | 22:DA:2328:A:C8    | 2.48                     | 0.48              |
| 22:DA:2330:G:N2    | 22:DA:2386:A:C4    | 2.81                     | 0.48              |
| 22:DA:2603:G:C5    | 22:DA:2604:U:C5    | 3.02                     | 0.48              |
| 22:DA:2624:G:H1'   | 48:D0:19:HIS:CE1   | 2.48                     | 0.48              |
| 22:DA:265:A:H4'    | 22:DA:266:G:OP1    | 2.13                     | 0.48              |
| 22:DA:693:A:C6     | 22:DA:694:U:C4     | 3.02                     | 0.48              |
| 22:DA:931:U:H4'    | 22:DA:932:U:OP2    | 2.14                     | 0.48              |
| 23:DB:58:A:H2'     | 23:DB:59:A:O4'     | 2.13                     | 0.48              |
| 24:DC:144:VAL:HB   | 24:DC:154:LEU:HB2  | 1.96                     | 0.48              |
| 24:DC:267:ILE:CG2  | 24:DC:267:ILE:O    | 2.61                     | 0.48              |
| 25:DD:101:PHE:HA   | 25:DD:104:VAL:HG13 | 1.95                     | 0.48              |
| 30:DI:80:LEU:HA    | 30:DI:84:ALA:HB2   | 1.94                     | 0.48              |
| 31:DJ:109:LEU:HD23 | 31:DJ:110:PRO:HD2  | 1.95                     | 0.48              |
| 31:DJ:84:ILE:HG13  | 31:DJ:84:ILE:O     | 2.13                     | 0.48              |
| 33:DL:82:LEU:HA    | 33:DL:85:VAL:HG13  | 1.94                     | 0.48              |
| 46:DY:46:VAL:O     | 46:DY:46:VAL:HG12  | 2.13                     | 0.48              |
| 1:AA:999:C:H2'     | 1:AA:1000:A:C8     | 2.48                     | 0.48              |
| 1:AA:104:G:C2      | 1:AA:105:G:C8      | 3.01                     | 0.48              |
| 1:AA:1095:U:H2'    | 1:AA:1096:C:O4'    | 2.13                     | 0.48              |
| 1:AA:1129:C:O2     | 1:AA:1130:A:N6     | 2.47                     | 0.48              |
| 1:AA:220:G:C5      | 1:AA:221:C:C5      | 3.01                     | 0.48              |
| 1:AA:455:G:C2      | 1:AA:478:A:C2      | 3.01                     | 0.48              |
| 1:AA:524:G:C6      | 1:AA:525:C:N4      | 2.81                     | 0.48              |
| 1:AA:1523:G:OP1    | 11:AK:128:ARG:NH2  | 2.46                     | 0.48              |
| 14:AN:46:LEU:HG    | 14:AN:47:LYS:N     | 2.29                     | 0.48              |
| 14:AN:4:GLN:O      | 14:AN:7:LYS:N      | 2.47                     | 0.48              |
| 50:B2:43:THR:O     | 50:B2:44:VAL:HB    | 2.13                     | 0.48              |
| 22:BA:1169:A:H2'   | 22:BA:1170:C:O4'   | 2.13                     | 0.48              |
| 22:BA:1359:A:N7    | 22:BA:1373:A:C2    | 2.81                     | 0.48              |
| 22:BA:1402:U:H2'   | 22:BA:1403:A:O5'   | 2.14                     | 0.48              |
| 22:BA:2322:A:H2'   | 22:BA:2323:G:O4'   | 2.12                     | 0.48              |
| 25:BD:108:ASP:OD1  | 25:BD:173:GLN:HG2  | 2.13                     | 0.48              |
| 25:BD:133:THR:HG23 | 25:BD:134:HIS:CG   | 2.49                     | 0.48              |
| 27:BF:28:VAL:O     | 27:BF:28:VAL:HG13  | 2.13                     | 0.48              |
| 33:BL:77:ILE:HD11  | 33:BL:101:ILE:CG2  | 2.43                     | 0.48              |
| 33:BL:109:LYS:HG2  | 33:BL:126:ARG:HB2  | 1.94                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:1029:U:O2     | 1:CA:1029:U:H2'    | 2.14                     | 0.48              |
| 1:CA:1328:C:H5''   | 13:CM:28:THR:HG21  | 1.94                     | 0.48              |
| 1:CA:238:A:O2'     | 1:CA:239:U:H5'     | 2.13                     | 0.48              |
| 1:CA:578:C:C2      | 1:CA:579:A:C8      | 3.01                     | 0.48              |
| 1:CA:582:C:C4      | 1:CA:760:G:C6      | 3.01                     | 0.48              |
| 5:CE:16:ILE:HD11   | 5:CE:38:VAL:HG23   | 1.95                     | 0.48              |
| 7:CG:92:ARG:NE     | 7:CG:93:PRO:HD2    | 2.28                     | 0.48              |
| 8:CH:86:TYR:O      | 8:CH:87:LYS:HD2    | 2.13                     | 0.48              |
| 10:CJ:57:VAL:HG13  | 10:CJ:58:ASN:N     | 2.28                     | 0.48              |
| 10:CJ:47:GLU:O     | 10:CJ:66:GLU:HA    | 2.13                     | 0.48              |
| 19:CS:34:TRP:HA    | 19:CS:52:HIS:HB2   | 1.96                     | 0.48              |
| 22:DA:126:A:C8     | 22:DA:127:A:C2     | 3.01                     | 0.48              |
| 22:DA:1369:G:C2    | 22:DA:1370:C:C6    | 3.01                     | 0.48              |
| 22:DA:1475:G:H4'   | 22:DA:1732:C:C5    | 2.49                     | 0.48              |
| 22:DA:1936:A:C8    | 22:DA:1945:G:C6    | 3.01                     | 0.48              |
| 22:DA:2345:G:C6    | 22:DA:2347:C:N4    | 2.81                     | 0.48              |
| 22:DA:2452:C:N4    | 22:DA:2453:A:C6    | 2.82                     | 0.48              |
| 22:DA:2478:A:C8    | 22:DA:2529:G:C6    | 3.01                     | 0.48              |
| 22:DA:2683:C:C5    | 22:DA:2684:U:C5    | 3.01                     | 0.48              |
| 22:DA:2845:U:H5''  | 37:DP:52:ASN:O     | 2.14                     | 0.48              |
| 22:DA:487:C:N4     | 22:DA:488:G:C6     | 2.82                     | 0.48              |
| 22:DA:83:A:C2      | 22:DA:103:A:N7     | 2.82                     | 0.48              |
| 24:DC:252:THR:HG22 | 24:DC:253:LYS:N    | 2.27                     | 0.48              |
| 25:DD:148:GLN:CD   | 25:DD:148:GLN:N    | 2.67                     | 0.48              |
| 26:DE:84:THR:O     | 26:DE:85:PHE:CG    | 2.67                     | 0.48              |
| 30:DI:90:SER:HB3   | 30:DI:93:PRO:HG3   | 1.94                     | 0.48              |
| 34:DM:120:ALA:O    | 34:DM:124:LEU:HD23 | 2.14                     | 0.48              |
| 44:DW:45:PHE:CG    | 44:DW:80:ILE:HD11  | 2.48                     | 0.48              |
| 1:AA:1181:G:C2     | 1:AA:1182:G:N2     | 2.82                     | 0.48              |
| 1:AA:1350:A:C5     | 1:AA:1351:U:C4     | 3.02                     | 0.48              |
| 1:AA:418:C:N4      | 57:AA:1718:HOH:O   | 2.46                     | 0.48              |
| 1:AA:736:C:H2'     | 1:AA:737:C:C6      | 2.49                     | 0.48              |
| 2:AB:173:ILE:HG23  | 2:AB:183:VAL:HG11  | 1.95                     | 0.48              |
| 2:AB:28:LYS:N      | 2:AB:29:PRO:CD     | 2.76                     | 0.48              |
| 3:AC:60:PRO:O      | 3:AC:61:ALA:C      | 2.52                     | 0.48              |
| 5:AE:81:LEU:N      | 5:AE:81:LEU:HD13   | 2.29                     | 0.48              |
| 1:AA:1250:A:H4'    | 9:AI:70:GLY:N      | 2.28                     | 0.48              |
| 12:AL:86:ARG:HA    | 12:AL:94:ARG:HA    | 1.95                     | 0.48              |
| 17:AQ:30:LYS:HG2   | 17:AQ:37:PHE:CZ    | 2.48                     | 0.48              |
| 22:BA:2742:G:OP1   | 52:B4:36:ARG:HD3   | 2.13                     | 0.48              |
| 22:BA:102:U:C2     | 46:BY:2:LYS:HE3    | 2.49                     | 0.48              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 22:BA:1413:A:O2'   | 22:BA:1414:C:H5'  | 2.14                     | 0.48              |
| 22:BA:1916:A:N9    | 22:BA:1917:U:H1'  | 2.27                     | 0.48              |
| 22:BA:2187:U:H2'   | 22:BA:2188:U:H1'  | 1.95                     | 0.48              |
| 22:BA:2669:G:C2'   | 22:BA:2670:A:H5'  | 2.44                     | 0.48              |
| 22:BA:2678:C:H2'   | 22:BA:2679:A:O4'  | 2.13                     | 0.48              |
| 22:BA:2727:A:C2'   | 22:BA:2728:U:H5'  | 2.44                     | 0.48              |
| 22:BA:287:G:H2'    | 22:BA:288:U:C6    | 2.49                     | 0.48              |
| 22:BA:499:U:C4     | 22:BA:500:G:C6    | 3.02                     | 0.48              |
| 22:BA:657:U:H2'    | 22:BA:658:U:C6    | 2.48                     | 0.48              |
| 23:BB:17:C:H2'     | 23:BB:18:G:O4'    | 2.14                     | 0.48              |
| 57:BA:3778:HOH:O   | 31:BJ:39:LYS:HE3  | 2.14                     | 0.48              |
| 32:BK:107:LEU:O    | 32:BK:108:ARG:C   | 2.52                     | 0.48              |
| 34:BM:77:PRO:HG2   | 34:BM:80:VAL:CG2  | 2.44                     | 0.48              |
| 43:BV:13:GLY:O     | 43:BV:17:SER:OG   | 2.32                     | 0.48              |
| 1:CA:120:A:OP2     | 1:CA:120:A:H2'    | 2.13                     | 0.48              |
| 1:CA:158:G:C6      | 1:CA:159:G:C5     | 3.02                     | 0.48              |
| 1:CA:189:A:N6      | 1:CA:190:A:N1     | 2.61                     | 0.48              |
| 1:CA:211:G:O2'     | 1:CA:212:G:C4'    | 2.62                     | 0.48              |
| 1:CA:833:G:N2      | 1:CA:834:U:H1'    | 2.29                     | 0.48              |
| 2:CB:81:LYS:HG3    | 2:CB:91:PHE:CZ    | 2.48                     | 0.48              |
| 3:CC:121:THR:O     | 3:CC:125:GLU:OE2  | 2.31                     | 0.48              |
| 4:CD:107:PHE:O     | 4:CD:117:LEU:CD1  | 2.60                     | 0.48              |
| 7:CG:92:ARG:NE     | 7:CG:93:PRO:HD3   | 2.28                     | 0.48              |
| 17:CQ:38:ILE:CG2   | 17:CQ:39:LYS:N    | 2.77                     | 0.48              |
| 22:DA:1076:C:H1'   | 30:DI:93:PRO:HG2  | 1.96                     | 0.48              |
| 22:DA:1277:G:N3    | 35:DN:23:ASN:HB3  | 2.29                     | 0.48              |
| 22:DA:1373:A:N6    | 22:DA:1374:G:C2   | 2.82                     | 0.48              |
| 22:DA:1682:G:H2'   | 22:DA:1683:U:C6   | 2.48                     | 0.48              |
| 22:DA:1936:A:H3'   | 22:DA:1937:A:H5'  | 1.96                     | 0.48              |
| 22:DA:2209:G:C6    | 22:DA:2210:U:O4   | 2.67                     | 0.48              |
| 22:DA:250:G:H2'    | 22:DA:251:A:C8    | 2.49                     | 0.48              |
| 22:DA:449:A:H2'    | 22:DA:450:G:H5'   | 1.96                     | 0.48              |
| 22:DA:771:G:C6     | 22:DA:772:C:C5    | 3.02                     | 0.48              |
| 23:DB:39:A:N6      | 23:DB:44:G:C6     | 2.81                     | 0.48              |
| 24:DC:69:ARG:NH2   | 24:DC:116:ILE:CD1 | 2.76                     | 0.48              |
| 24:DC:147:LYS:O    | 24:DC:150:LYS:HB3 | 2.13                     | 0.48              |
| 25:DD:133:THR:HG23 | 25:DD:134:HIS:H   | 1.79                     | 0.48              |
| 26:DE:52:VAL:HG21  | 26:DE:81:GLY:HA2  | 1.95                     | 0.48              |
| 27:DF:122:PHE:CE1  | 27:DF:166:GLY:C   | 2.87                     | 0.48              |
| 33:DL:102:GLY:N    | 57:DL:301:HOH:O   | 2.47                     | 0.48              |
| 39:DR:80:ARG:O     | 39:DR:82:HIS:N    | 2.42                     | 0.48              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 29:DH:27:ARG:HE   | 45:DX:60:ASP:CG    | 2.16                     | 0.48              |
| 1:AA:1356:G:H2'   | 1:AA:1357:A:C8     | 2.49                     | 0.48              |
| 1:AA:451:A:C5'    | 16:AP:70:ARG:HH22  | 2.27                     | 0.48              |
| 1:AA:457:G:C5     | 1:AA:458:U:C5      | 3.02                     | 0.48              |
| 4:AD:75:TYR:OH    | 4:AD:97:ARG:NH1    | 2.46                     | 0.48              |
| 6:AF:66:ALA:HB1   | 6:AF:67:PRO:HD2    | 1.96                     | 0.48              |
| 7:AG:49:THR:O     | 7:AG:53:ARG:HB3    | 2.13                     | 0.48              |
| 11:AK:88:GLY:N    | 11:AK:114:THR:HG22 | 2.29                     | 0.48              |
| 1:AA:1492:A:OP1   | 12:AL:44:LYS:HA    | 2.14                     | 0.48              |
| 12:AL:86:ARG:CZ   | 12:AL:88:LYS:HB3   | 2.44                     | 0.48              |
| 22:BA:1079:C:C5   | 22:BA:1088:A:N1    | 2.82                     | 0.48              |
| 22:BA:1180:U:H2'  | 22:BA:1181:U:H5'   | 1.95                     | 0.48              |
| 22:BA:1248:G:OP1  | 38:BQ:2:ALA:HB3    | 2.13                     | 0.48              |
| 22:BA:1352:U:C2'  | 22:BA:1353:A:H5'   | 2.44                     | 0.48              |
| 22:BA:1796:U:H2'  | 22:BA:1797:G:H8    | 1.79                     | 0.48              |
| 22:BA:2173:A:C8   | 22:BA:2174:C:C5    | 3.02                     | 0.48              |
| 22:BA:2287:A:C5   | 22:BA:2289:G:C8    | 3.02                     | 0.48              |
| 22:BA:2435:A:H2'  | 22:BA:2436:G:O5'   | 2.14                     | 0.48              |
| 22:BA:2665:A:C2   | 22:BA:2666:C:N1    | 2.81                     | 0.48              |
| 22:BA:2887:A:H3'  | 22:BA:2888:C:H6    | 1.77                     | 0.48              |
| 22:BA:277:G:C2'   | 22:BA:361:G:O6     | 2.61                     | 0.48              |
| 22:BA:404:A:C2'   | 22:BA:405:U:OP2    | 2.62                     | 0.48              |
| 22:BA:655:A:H4'   | 22:BA:656:G:OP1    | 2.12                     | 0.48              |
| 27:BF:68:THR:N    | 27:BF:86:GLY:O     | 2.45                     | 0.48              |
| 28:BG:141:ILE:C   | 28:BG:141:ILE:HD12 | 2.33                     | 0.48              |
| 28:BG:69:ARG:C    | 28:BG:69:ARG:HD3   | 2.33                     | 0.48              |
| 33:BL:132:ARG:HG3 | 33:BL:142:ILE:HD12 | 1.96                     | 0.48              |
| 38:BQ:21:ALA:HB1  | 38:BQ:28:ARG:O     | 2.13                     | 0.48              |
| 39:BR:48:LYS:O    | 39:BR:49:ILE:C     | 2.51                     | 0.48              |
| 1:CA:1160:G:O2'   | 1:CA:1161:C:P      | 2.72                     | 0.48              |
| 1:CA:1404:C:H2'   | 1:CA:1405:G:C8     | 2.48                     | 0.48              |
| 1:CA:32:A:N1      | 1:CA:33:A:C6       | 2.82                     | 0.48              |
| 1:CA:811:C:H4'    | 1:CA:900:A:N6      | 2.29                     | 0.48              |
| 4:CD:139:PRO:O    | 4:CD:140:ASN:HB2   | 2.14                     | 0.48              |
| 4:CD:202:GLU:OE1  | 5:CE:105:ILE:HG23  | 2.13                     | 0.48              |
| 11:CK:82:LEU:HD22 | 11:CK:105:PHE:HB3  | 1.95                     | 0.48              |
| 22:DA:1095:A:C2   | 30:DI:30:GLN:HB3   | 2.49                     | 0.48              |
| 22:DA:1262:A:N3   | 22:DA:1262:A:H2'   | 2.27                     | 0.48              |
| 22:DA:1401:G:C6   | 22:DA:1402:U:C4    | 3.01                     | 0.48              |
| 22:DA:1523:U:H3'  | 22:DA:1524:G:H8    | 1.78                     | 0.48              |
| 22:DA:1831:G:C5   | 22:DA:1832:C:C4    | 3.02                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:DA:2094:A:C2    | 22:DA:2196:C:C2    | 3.01                     | 0.48              |
| 22:DA:2093:G:C6    | 22:DA:2225:A:C8    | 3.02                     | 0.48              |
| 22:DA:67:U:H2'     | 22:DA:68:G:O4'     | 2.14                     | 0.48              |
| 24:DC:157:SER:HB2  | 24:DC:160:THR:HG21 | 1.95                     | 0.48              |
| 25:DD:146:ILE:HG13 | 25:DD:146:ILE:O    | 2.13                     | 0.48              |
| 35:DN:114:GLU:OE2  | 35:DN:118:ARG:HD2  | 2.13                     | 0.48              |
| 40:DS:61:ASN:O     | 40:DS:62:ASP:CB    | 2.61                     | 0.48              |
| 1:AA:1000:A:C2     | 1:AA:1041:G:C2     | 3.01                     | 0.48              |
| 1:AA:119:A:C4      | 1:AA:240:G:N7      | 2.81                     | 0.48              |
| 1:AA:126:G:H2'     | 1:AA:127:G:O4'     | 2.14                     | 0.48              |
| 1:AA:1406:U:H2'    | 1:AA:1407:C:C5'    | 2.44                     | 0.48              |
| 1:AA:2:A:N6        | 1:AA:3:A:N1        | 2.61                     | 0.48              |
| 1:AA:404:G:H4'     | 1:AA:439:U:O2      | 2.14                     | 0.48              |
| 1:AA:47:C:O2       | 1:AA:49:U:C5       | 2.66                     | 0.48              |
| 1:AA:702:A:H3'     | 1:AA:703:G:H5'     | 1.94                     | 0.48              |
| 8:AH:10:MET:CE     | 8:AH:33:LYS:HD3    | 2.44                     | 0.48              |
| 8:AH:83:LEU:HD22   | 8:AH:83:LEU:C      | 2.34                     | 0.48              |
| 9:AI:50:GLN:O      | 9:AI:52:LEU:N      | 2.46                     | 0.48              |
| 12:AL:63:VAL:HG21  | 12:AL:95:TYR:CE2   | 2.49                     | 0.48              |
| 14:AN:16:LEU:HD23  | 14:AN:16:LEU:N     | 2.29                     | 0.48              |
| 22:BA:1045:C:C4'   | 22:BA:1046:A:H5'   | 2.44                     | 0.48              |
| 22:BA:1187:G:P     | 57:BA:3372:HOH:O   | 2.71                     | 0.48              |
| 22:BA:1876:A:C2    | 22:BA:1877:A:C4    | 3.02                     | 0.48              |
| 22:BA:1912:A:C2    | 22:BA:1919:A:C5    | 3.01                     | 0.48              |
| 22:BA:2308:G:H5''  | 22:BA:2309:A:OP2   | 2.14                     | 0.48              |
| 22:BA:2344:U:H4'   | 22:BA:2345:G:OP1   | 2.13                     | 0.48              |
| 22:BA:1672:A:C2    | 22:BA:2582:G:H5'   | 2.49                     | 0.48              |
| 22:BA:613:A:C8     | 22:BA:616:A:C2     | 3.02                     | 0.48              |
| 22:BA:64:A:C5      | 22:BA:65:U:C4      | 3.02                     | 0.48              |
| 22:BA:2052:A:H4'   | 25:BD:148:GLN:O    | 2.13                     | 0.48              |
| 27:BF:174:ASP:O    | 27:BF:175:PHE:O    | 2.31                     | 0.48              |
| 29:BH:103:VAL:HG21 | 29:BH:132:PHE:CZ   | 2.49                     | 0.48              |
| 29:BH:135:HIS:CD2  | 29:BH:137:GLU:HG3  | 2.48                     | 0.48              |
| 39:BR:49:ILE:HG22  | 39:BR:52:PRO:C     | 2.33                     | 0.48              |
| 1:CA:1001:C:H2'    | 1:CA:1002:G:C8     | 2.49                     | 0.48              |
| 1:CA:1104:G:C6     | 1:CA:1105:A:C5     | 3.02                     | 0.48              |
| 1:CA:1298:U:O2     | 1:CA:1298:U:H2'    | 2.13                     | 0.48              |
| 1:CA:1408:A:C2     | 1:CA:1494:G:N3     | 2.82                     | 0.48              |
| 1:CA:17:U:H2'      | 1:CA:18:C:H6       | 1.76                     | 0.48              |
| 1:CA:29:U:H5'      | 1:CA:296:U:OP1     | 2.14                     | 0.48              |
| 1:CA:582:C:C2      | 1:CA:760:G:N1      | 2.81                     | 0.48              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:722:G:N3      | 1:CA:722:G:H3'     | 2.29                     | 0.48              |
| 1:CA:756:C:H2'     | 1:CA:757:U:C5'     | 2.43                     | 0.48              |
| 1:CA:756:C:C2      | 1:CA:757:U:C6      | 3.01                     | 0.48              |
| 1:CA:829:G:C6      | 1:CA:858:G:C2      | 3.01                     | 0.48              |
| 4:CD:151:LYS:C     | 4:CD:152:GLN:OE1   | 2.52                     | 0.48              |
| 4:CD:53:VAL:HG23   | 4:CD:54:GLN:N      | 2.29                     | 0.48              |
| 1:CA:1377:A:C6     | 7:CG:7:ILE:HD12    | 2.49                     | 0.48              |
| 12:CL:44:LYS:HD3   | 12:CL:44:LYS:N     | 2.27                     | 0.48              |
| 13:CM:27:LYS:O     | 13:CM:27:LYS:CD    | 2.62                     | 0.48              |
| 14:CN:24:ARG:CZ    | 14:CN:51:LEU:HD11  | 2.44                     | 0.48              |
| 17:CQ:52:GLU:HG2   | 17:CQ:53:CYS:N     | 2.29                     | 0.48              |
| 48:D0:28:LEU:HD23  | 48:D0:37:LYS:HB3   | 1.96                     | 0.48              |
| 22:DA:197:A:N3     | 22:DA:197:A:H2'    | 2.29                     | 0.48              |
| 22:DA:2519:U:C6    | 22:DA:2542:A:N6    | 2.82                     | 0.48              |
| 22:DA:2562:U:H2'   | 22:DA:2563:U:H5'   | 1.95                     | 0.48              |
| 22:DA:2736:A:C4    | 22:DA:2737:G:C8    | 3.01                     | 0.48              |
| 22:DA:228:C:N4     | 22:DA:417:C:O2     | 2.47                     | 0.48              |
| 22:DA:477:A:H2'    | 22:DA:478:A:O5'    | 2.14                     | 0.48              |
| 24:DC:124:ILE:HG22 | 24:DC:124:ILE:O    | 2.14                     | 0.48              |
| 24:DC:108:LYS:HA   | 24:DC:196:GLY:CA   | 2.44                     | 0.48              |
| 26:DE:150:THR:O    | 26:DE:172:ALA:HB2  | 2.13                     | 0.48              |
| 28:DG:158:LYS:C    | 28:DG:160:LYS:N    | 2.67                     | 0.48              |
| 45:DX:51:VAL:HG23  | 45:DX:52:SER:N     | 2.29                     | 0.48              |
| 22:DA:920:A:OP1    | 47:DZ:19:LYS:HE3   | 2.14                     | 0.48              |
| 1:AA:17:U:H2'      | 1:AA:18:C:C6       | 2.49                     | 0.48              |
| 3:AC:7:PRO:HD2     | 3:AC:184:TYR:CD2   | 2.48                     | 0.48              |
| 5:AE:144:LEU:O     | 5:AE:147:MET:HB3   | 2.13                     | 0.48              |
| 7:AG:72:THR:HA     | 7:AG:96:ARG:NH1    | 2.29                     | 0.48              |
| 21:AU:10:GLU:HG3   | 21:AU:11:PRO:HD3   | 1.96                     | 0.48              |
| 21:AU:25:LYS:O     | 21:AU:29:LEU:HB3   | 2.14                     | 0.48              |
| 22:BA:1009:A:H8    | 22:BA:1009:A:O5'   | 1.96                     | 0.48              |
| 22:BA:1378:A:O2'   | 57:BA:3753:HOH:O   | 2.20                     | 0.48              |
| 22:BA:2553:G:H5''  | 22:BA:2554:U:OP2   | 2.14                     | 0.48              |
| 25:BD:101:PHE:O    | 25:BD:102:ALA:C    | 2.52                     | 0.48              |
| 30:BI:108:GLU:OE2  | 30:BI:109:ILE:HG13 | 2.13                     | 0.48              |
| 32:BK:63:VAL:HG12  | 32:BK:107:LEU:HD11 | 1.96                     | 0.48              |
| 34:BM:77:PRO:HG2   | 34:BM:80:VAL:HG21  | 1.96                     | 0.48              |
| 35:BN:49:GLU:N     | 35:BN:50:PRO:CD    | 2.77                     | 0.48              |
| 45:BX:33:LEU:O     | 45:BX:34:HIS:CG    | 2.66                     | 0.48              |
| 45:BX:78:TYR:CG    | 45:BX:78:TYR:OXT   | 2.67                     | 0.48              |
| 1:CA:1478:U:H2'    | 1:CA:1479:C:H6     | 1.79                     | 0.48              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CA:202:G:H2'    | 1:CA:203:G:O4'    | 2.14                     | 0.48              |
| 1:CA:203:G:N2     | 1:CA:215:C:C2     | 2.82                     | 0.48              |
| 1:CA:555:U:H2'    | 1:CA:556:C:C6     | 2.49                     | 0.48              |
| 1:CA:671:G:N1     | 1:CA:672:U:C2     | 2.81                     | 0.48              |
| 5:CE:20:ARG:HG2   | 5:CE:20:ARG:O     | 2.14                     | 0.48              |
| 17:CQ:19:LYS:CD   | 17:CQ:49:GLU:HA   | 2.44                     | 0.48              |
| 51:D3:26:HIS:CE1  | 51:D3:48:ALA:HB2  | 2.48                     | 0.48              |
| 22:DA:1255:U:H2'  | 22:DA:1256:G:OP1  | 2.14                     | 0.48              |
| 22:DA:1280:G:C6   | 22:DA:1281:G:C5   | 3.02                     | 0.48              |
| 22:DA:134:G:N2    | 22:DA:146:A:C2    | 2.82                     | 0.48              |
| 22:DA:1403:A:H2'  | 22:DA:1404:C:C6   | 2.48                     | 0.48              |
| 22:DA:1869:G:C3'  | 22:DA:1870:C:H5'  | 2.44                     | 0.48              |
| 22:DA:1931:U:C2   | 22:DA:1932:A:C8   | 3.02                     | 0.48              |
| 22:DA:2308:G:O6   | 22:DA:2311:A:N7   | 2.47                     | 0.48              |
| 22:DA:2283:C:C4   | 22:DA:2389:G:C4   | 3.02                     | 0.48              |
| 22:DA:2694:G:C5   | 22:DA:2695:U:C5   | 3.01                     | 0.48              |
| 22:DA:2699:C:H2'  | 22:DA:2700:A:O4'  | 2.14                     | 0.48              |
| 22:DA:284:U:H2'   | 22:DA:284:U:O2    | 2.12                     | 0.48              |
| 22:DA:228:C:N3    | 22:DA:418:C:C4'   | 2.77                     | 0.48              |
| 22:DA:33:C:O2     | 22:DA:447:A:N6    | 2.46                     | 0.48              |
| 22:DA:570:G:H2'   | 22:DA:571:U:H5'   | 1.94                     | 0.48              |
| 22:DA:696:G:C6    | 22:DA:767:U:C2    | 3.02                     | 0.48              |
| 22:DA:856:G:C2    | 22:DA:922:C:C2    | 3.01                     | 0.48              |
| 25:DD:104:VAL:O   | 25:DD:105:LYS:HB2 | 2.13                     | 0.48              |
| 26:DE:97:ASN:HB2  | 26:DE:100:MET:SD  | 2.54                     | 0.48              |
| 33:DL:61:LEU:O    | 51:D3:13:ARG:NH2  | 2.44                     | 0.48              |
| 22:DA:1198:U:O2   | 38:DQ:4:VAL:HG11  | 2.13                     | 0.48              |
| 42:DU:83:VAL:CG1  | 42:DU:84:GLY:N    | 2.77                     | 0.48              |
| 1:AA:102:G:C2     | 1:AA:103:U:C5     | 3.01                     | 0.48              |
| 1:AA:1163:A:C2    | 1:AA:1174:G:C2    | 3.02                     | 0.48              |
| 1:AA:1190:G:P     | 3:AC:5:VAL:HG12   | 2.54                     | 0.48              |
| 1:AA:1346:A:N1    | 1:AA:1374:A:H5''  | 2.28                     | 0.48              |
| 1:AA:601:G:C6     | 1:AA:602:A:C6     | 3.02                     | 0.48              |
| 1:AA:626:G:C6     | 1:AA:627:G:C5     | 3.02                     | 0.48              |
| 1:AA:728:A:C6     | 1:AA:729:A:C6     | 3.02                     | 0.48              |
| 2:AB:164:ILE:HG12 | 2:AB:165:ASP:N    | 2.28                     | 0.48              |
| 2:AB:206:ALA:O    | 2:AB:208:ARG:N    | 2.47                     | 0.48              |
| 4:AD:116:GLN:HG3  | 4:AD:120:HIS:CE1  | 2.48                     | 0.48              |
| 7:AG:55:GLY:C     | 7:AG:57:SER:N     | 2.66                     | 0.48              |
| 10:AJ:52:LEU:HB2  | 14:AN:81:ARG:CD   | 2.44                     | 0.48              |
| 12:AL:22:PRO:C    | 12:AL:24:LEU:N    | 2.68                     | 0.48              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 13:AM:11:ASP:O     | 13:AM:12:HIS:CB   | 2.62                     | 0.48              |
| 18:AR:25:ASP:C     | 18:AR:27:ALA:N    | 2.67                     | 0.48              |
| 1:AA:1314:C:H41    | 19:AS:4:SER:HA    | 1.79                     | 0.48              |
| 13:AM:83:LEU:HD21  | 19:AS:65:GLU:CG   | 2.44                     | 0.48              |
| 22:BA:141:G:N1     | 41:BT:1:MET:HE1   | 2.28                     | 0.48              |
| 22:BA:1501:G:O2'   | 22:BA:1502:A:H5'  | 2.14                     | 0.48              |
| 22:BA:1916:A:H2'   | 22:BA:1917:U:C2'  | 2.44                     | 0.48              |
| 22:BA:2339:C:H2'   | 22:BA:2340:A:H8   | 1.78                     | 0.48              |
| 22:BA:877:A:O2'    | 22:BA:900:A:N6    | 2.46                     | 0.48              |
| 22:BA:998:C:OP1    | 57:BA:3363:HOH:O  | 2.20                     | 0.48              |
| 23:BB:14:U:OP2     | 23:BB:71:C:H5'    | 2.14                     | 0.48              |
| 24:BC:162:VAL:HG11 | 24:BC:174:LEU:HB3 | 1.95                     | 0.48              |
| 22:BA:1805:A:H1'   | 24:BC:50:THR:O    | 2.14                     | 0.48              |
| 26:BE:111:GLU:CG   | 26:BE:114:ARG:NH1 | 2.77                     | 0.48              |
| 27:BF:103:LEU:O    | 27:BF:108:VAL:HB  | 2.13                     | 0.48              |
| 27:BF:40:VAL:CG1   | 27:BF:43:ALA:HB3  | 2.43                     | 0.48              |
| 27:BF:73:SER:HB2   | 27:BF:81:GLN:N    | 2.29                     | 0.48              |
| 31:BJ:17:VAL:HG22  | 31:BJ:55:ILE:HB   | 1.96                     | 0.48              |
| 36:BO:83:LEU:HD23  | 36:BO:83:LEU:N    | 2.28                     | 0.48              |
| 37:BP:31:TRP:CD2   | 37:BP:40:LEU:HD12 | 2.48                     | 0.48              |
| 1:CA:1511:G:C5     | 1:CA:1512:U:C5    | 3.01                     | 0.48              |
| 1:CA:577:G:C2      | 1:CA:578:C:C5     | 3.02                     | 0.48              |
| 1:CA:690:G:H2'     | 1:CA:691:G:O4'    | 2.14                     | 0.48              |
| 3:CC:36:ASP:O      | 3:CC:40:ARG:HG3   | 2.13                     | 0.48              |
| 4:CD:107:PHE:CD1   | 4:CD:107:PHE:N    | 2.80                     | 0.48              |
| 5:CE:83:HIS:NE2    | 8:CH:96:MET:CE    | 2.77                     | 0.48              |
| 8:CH:21:ASN:O      | 8:CH:23:ALA:N     | 2.47                     | 0.48              |
| 1:CA:643:C:C5'     | 8:CH:32:LEU:HD22  | 2.44                     | 0.48              |
| 52:D4:16:ILE:HD13  | 52:D4:25:VAL:HG22 | 1.96                     | 0.48              |
| 22:DA:1250:G:C5'   | 38:DQ:6:ARG:HD2   | 2.44                     | 0.48              |
| 22:DA:585:G:C2     | 22:DA:1256:G:C6   | 3.01                     | 0.48              |
| 22:DA:1356:G:N2    | 22:DA:1357:C:H1'  | 2.29                     | 0.48              |
| 22:DA:1555:G:N2    | 22:DA:1556:C:H1'  | 2.29                     | 0.48              |
| 22:DA:2333:A:OP2   | 44:DW:77:ARG:NH2  | 2.39                     | 0.48              |
| 22:DA:2345:G:H4'   | 22:DA:2346:A:H5'' | 1.96                     | 0.48              |
| 22:DA:2373:G:C2    | 22:DA:2374:C:C2   | 3.01                     | 0.48              |
| 22:DA:241:A:C6     | 22:DA:255:A:H5''  | 2.49                     | 0.48              |
| 22:DA:2808:G:N2    | 22:DA:2891:U:C6   | 2.82                     | 0.48              |
| 22:DA:2842:G:H2'   | 22:DA:2843:G:O4'  | 2.13                     | 0.48              |
| 22:DA:301:G:H5'    | 22:DA:334:C:O2    | 2.13                     | 0.48              |
| 22:DA:382:A:N1     | 22:DA:383:C:C2    | 2.82                     | 0.48              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:DA:389:G:C2    | 22:DA:2413:G:H1'   | 2.49                     | 0.48              |
| 22:DA:426:C:H2'   | 22:DA:427:U:O4'    | 2.13                     | 0.48              |
| 22:DA:749:A:C5    | 22:DA:750:A:C8     | 3.02                     | 0.48              |
| 22:DA:777:G:N2    | 22:DA:778:G:C8     | 2.82                     | 0.48              |
| 22:DA:909:A:C6    | 22:DA:912:C:C2     | 3.02                     | 0.48              |
| 22:DA:915:C:N4    | 22:DA:916:G:C6     | 2.82                     | 0.48              |
| 26:DE:59:PRO:HB2  | 26:DE:70:SER:OG    | 2.13                     | 0.48              |
| 22:DA:1665:A:H5'' | 32:DK:66:LYS:HG3   | 1.96                     | 0.48              |
| 38:DQ:76:TYR:CZ   | 38:DQ:80:ILE:HG13  | 2.49                     | 0.48              |
| 42:DU:16:GLY:O    | 42:DU:17:LYS:HB2   | 2.14                     | 0.48              |
| 1:AA:116:A:C4     | 1:AA:117:G:C8      | 3.02                     | 0.47              |
| 1:AA:259:G:H2'    | 1:AA:260:G:O4'     | 2.15                     | 0.47              |
| 1:AA:553:A:O2'    | 1:AA:554:A:H5'     | 2.13                     | 0.47              |
| 1:AA:65:A:C5      | 1:AA:381:C:C4      | 3.01                     | 0.47              |
| 1:AA:676:A:H5''   | 11:AK:115:PRO:HB3  | 1.96                     | 0.47              |
| 1:AA:72:A:H2'     | 1:AA:73:C:H5'      | 1.95                     | 0.47              |
| 1:AA:74:A:H1'     | 1:AA:97:G:N2       | 2.28                     | 0.47              |
| 4:AD:17:THR:HG23  | 4:AD:18:ASP:N      | 2.28                     | 0.47              |
| 1:AA:430:A:OP1    | 4:AD:9:LEU:HB2     | 2.13                     | 0.47              |
| 10:AJ:57:VAL:O    | 10:AJ:58:ASN:CB    | 2.63                     | 0.47              |
| 10:AJ:59:LYS:HD2  | 10:AJ:60:ASP:N     | 2.29                     | 0.47              |
| 13:AM:11:ASP:O    | 13:AM:12:HIS:ND1   | 2.47                     | 0.47              |
| 17:AQ:12:VAL:O    | 17:AQ:13:VAL:CB    | 2.61                     | 0.47              |
| 53:B5:218:THR:O   | 53:B5:219:MET:CB   | 2.60                     | 0.47              |
| 22:BA:1494:A:C2   | 22:BA:1495:A:N9    | 2.83                     | 0.47              |
| 22:BA:1850:G:C5   | 22:BA:1851:U:C4    | 3.02                     | 0.47              |
| 22:BA:197:A:N6    | 22:BA:2430:A:H2'   | 2.29                     | 0.47              |
| 22:BA:2131:U:OP2  | 22:BA:2132:U:C5    | 2.67                     | 0.47              |
| 23:BB:39:A:C2     | 23:BB:44:G:C4      | 3.02                     | 0.47              |
| 26:BE:176:ASP:OD1 | 26:BE:178:VAL:HG13 | 2.14                     | 0.47              |
| 30:BI:28:LEU:HG   | 30:BI:35:ILE:HD12  | 1.95                     | 0.47              |
| 31:BJ:57:LEU:HD22 | 31:BJ:128:ASN:HA   | 1.96                     | 0.47              |
| 35:BN:82:GLU:O    | 35:BN:85:PRO:HG2   | 2.13                     | 0.47              |
| 39:BR:14:VAL:HG13 | 39:BR:15:SER:N     | 2.29                     | 0.47              |
| 1:CA:1040:U:H2'   | 1:CA:1041:G:C8     | 2.49                     | 0.47              |
| 1:CA:1255:G:N1    | 1:CA:1279:G:N7     | 2.62                     | 0.47              |
| 1:CA:1273:C:H2'   | 1:CA:1274:A:O4'    | 2.13                     | 0.47              |
| 1:CA:1307:U:C4    | 1:CA:1308:U:C5     | 3.02                     | 0.47              |
| 1:CA:1423:G:H2'   | 1:CA:1424:U:O4'    | 2.14                     | 0.47              |
| 1:CA:407:U:H2'    | 1:CA:408:A:C8      | 2.49                     | 0.47              |
| 1:CA:457:G:C6     | 1:CA:458:U:N3      | 2.82                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:477:C:H2'     | 1:CA:478:A:C8      | 2.50                     | 0.47              |
| 1:CA:673:A:H2'     | 1:CA:674:G:C8      | 2.48                     | 0.47              |
| 2:CB:123:ASP:O     | 2:CB:124:GLY:C     | 2.51                     | 0.47              |
| 6:CF:81:ASN:OD1    | 6:CF:83:ALA:N      | 2.45                     | 0.47              |
| 10:CJ:91:ASP:O     | 10:CJ:92:LEU:HB2   | 2.14                     | 0.47              |
| 11:CK:107:ILE:HD13 | 11:CK:107:ILE:C    | 2.33                     | 0.47              |
| 11:CK:58:SER:O     | 11:CK:91:PRO:HG3   | 2.14                     | 0.47              |
| 51:D3:24:HIS:CE1   | 51:D3:48:ALA:HB3   | 2.49                     | 0.47              |
| 22:DA:1208:C:C4    | 22:DA:1209:U:C5    | 3.02                     | 0.47              |
| 22:DA:1339:G:O4'   | 22:DA:1393:A:C2    | 2.67                     | 0.47              |
| 22:DA:1324:G:O4'   | 22:DA:1616:A:N6    | 2.46                     | 0.47              |
| 22:DA:1682:G:C2    | 22:DA:1757:A:O4'   | 2.67                     | 0.47              |
| 22:DA:1809:A:C6    | 22:DA:1810:A:C6    | 3.02                     | 0.47              |
| 22:DA:1819:A:H5''  | 24:DC:157:SER:HB2  | 1.96                     | 0.47              |
| 22:DA:183:C:C5     | 22:DA:184:C:C5     | 3.01                     | 0.47              |
| 22:DA:2024:G:OP2   | 22:DA:2034:U:H4'   | 2.14                     | 0.47              |
| 22:DA:45:G:H2'     | 22:DA:215:G:N7     | 2.29                     | 0.47              |
| 22:DA:228:C:H4'    | 22:DA:229:C:H5''   | 1.96                     | 0.47              |
| 22:DA:228:C:O2     | 22:DA:418:C:H4'    | 2.14                     | 0.47              |
| 22:DA:2464:G:H2'   | 22:DA:2465:C:O4'   | 2.13                     | 0.47              |
| 22:DA:302:C:C2     | 22:DA:303:G:C8     | 3.01                     | 0.47              |
| 23:DB:81:G:C6      | 23:DB:82:U:C4      | 3.02                     | 0.47              |
| 24:DC:3:VAL:HG11   | 24:DC:202:LEU:HD23 | 1.95                     | 0.47              |
| 26:DE:149:ILE:HG21 | 26:DE:188:MET:SD   | 2.54                     | 0.47              |
| 30:DI:101:ILE:O    | 30:DI:102:SER:CB   | 2.62                     | 0.47              |
| 41:DT:35:ALA:O     | 41:DT:36:LYS:C     | 2.52                     | 0.47              |
| 41:DT:64:LYS:HA    | 41:DT:79:ASP:OD1   | 2.14                     | 0.47              |
| 42:DU:82:ARG:CZ    | 42:DU:82:ARG:HB2   | 2.43                     | 0.47              |
| 1:AA:1157:A:N7     | 1:AA:1180:A:C6     | 2.82                     | 0.47              |
| 1:AA:1306:A:C5     | 1:AA:1307:U:C5     | 3.02                     | 0.47              |
| 1:AA:1406:U:H2'    | 1:AA:1407:C:H5'    | 1.96                     | 0.47              |
| 1:AA:411:A:C6      | 1:AA:429:U:C4      | 3.02                     | 0.47              |
| 1:AA:518:C:H5      | 1:AA:530:G:OP2     | 1.97                     | 0.47              |
| 1:AA:791:G:C5      | 1:AA:792:A:N7      | 2.82                     | 0.47              |
| 4:AD:170:TRP:CD2   | 4:AD:186:PRO:HG3   | 2.49                     | 0.47              |
| 9:AI:58:VAL:O      | 9:AI:59:GLU:CG     | 2.63                     | 0.47              |
| 9:AI:26:GLY:N      | 9:AI:59:GLU:HA     | 2.29                     | 0.47              |
| 11:AK:76:GLU:N     | 11:AK:76:GLU:OE2   | 2.47                     | 0.47              |
| 17:AQ:60:GLU:OE1   | 17:AQ:77:ARG:HD3   | 2.14                     | 0.47              |
| 22:BA:1932:A:H5''  | 22:BA:1933:G:OP2   | 2.14                     | 0.47              |
| 11:AK:13:ARG:CZ    | 22:BA:2142:A:OP1   | 2.61                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:BA:2228:G:H2'  | 22:BA:2229:U:C6   | 2.50                     | 0.47              |
| 22:BA:416:U:C4    | 22:BA:417:C:C4    | 3.02                     | 0.47              |
| 22:BA:609:A:H2'   | 22:BA:610:C:O4'   | 2.14                     | 0.47              |
| 24:BC:31:ALA:HB3  | 24:BC:32:PRO:HD3  | 1.96                     | 0.47              |
| 28:BG:126:PRO:HG2 | 28:BG:130:GLU:HB3 | 1.95                     | 0.47              |
| 29:BH:116:ARG:O   | 29:BH:118:PRO:HD3 | 2.14                     | 0.47              |
| 47:BZ:45:ARG:NH1  | 47:BZ:59:GLU:OE1  | 2.46                     | 0.47              |
| 1:CA:1084:G:H5'   | 1:CA:1102:A:OP2   | 2.14                     | 0.47              |
| 1:CA:1388:C:N3    | 1:CA:1389:C:C5    | 2.83                     | 0.47              |
| 1:CA:143:A:H5'    | 1:CA:144:G:C5'    | 2.44                     | 0.47              |
| 1:CA:1460:C:C4    | 1:CA:1461:G:C5    | 3.02                     | 0.47              |
| 1:CA:374:A:N3     | 1:CA:375:U:C6     | 2.83                     | 0.47              |
| 1:CA:38:G:C2      | 1:CA:397:A:C2     | 3.02                     | 0.47              |
| 1:CA:476:U:O2'    | 1:CA:477:C:H5'    | 2.13                     | 0.47              |
| 1:CA:609:A:H2'    | 1:CA:610:U:H5'    | 1.96                     | 0.47              |
| 1:CA:704:A:C6     | 1:CA:705:G:C4     | 3.03                     | 0.47              |
| 1:CA:755:G:C2     | 1:CA:756:C:C6     | 3.02                     | 0.47              |
| 1:CA:933:G:OP2    | 7:CG:3:ARG:HB3    | 2.14                     | 0.47              |
| 1:CA:983:A:N3     | 1:CA:983:A:C2'    | 2.78                     | 0.47              |
| 1:CA:992:U:C2     | 1:CA:1043:G:N7    | 2.83                     | 0.47              |
| 2:CB:15:HIS:O     | 2:CB:16:PHE:C     | 2.52                     | 0.47              |
| 2:CB:35:ARG:O     | 2:CB:38:VAL:N     | 2.45                     | 0.47              |
| 7:CG:92:ARG:CZ    | 7:CG:93:PRO:HD3   | 2.45                     | 0.47              |
| 9:CI:81:HIS:O     | 9:CI:85:ARG:HB2   | 2.13                     | 0.47              |
| 1:CA:1216:A:OP1   | 14:CN:5:SER:CB    | 2.63                     | 0.47              |
| 22:DA:1138:G:H2'  | 22:DA:1139:G:O4'  | 2.14                     | 0.47              |
| 22:DA:1365:A:H2'  | 22:DA:1365:A:N3   | 2.27                     | 0.47              |
| 22:DA:1668:A:C4   | 22:DA:1674:G:C8   | 3.01                     | 0.47              |
| 22:DA:1692:U:O2'  | 22:DA:1693:U:H2'  | 2.14                     | 0.47              |
| 22:DA:1735:A:N1   | 22:DA:1736:U:C2   | 2.82                     | 0.47              |
| 22:DA:2123:G:C2   | 22:DA:2176:A:C2   | 3.02                     | 0.47              |
| 22:DA:218:A:C2    | 22:DA:219:A:C4    | 3.02                     | 0.47              |
| 22:DA:2305:U:C4   | 22:DA:2306:C:C4   | 3.02                     | 0.47              |
| 22:DA:415:A:C2    | 22:DA:2409:G:C6   | 3.02                     | 0.47              |
| 22:DA:2282:G:C5   | 22:DA:2425:A:N1   | 2.82                     | 0.47              |
| 22:DA:2513:A:C6   | 22:DA:2514:U:C4   | 3.02                     | 0.47              |
| 22:DA:430:A:H2'   | 22:DA:431:U:H5'   | 1.96                     | 0.47              |
| 22:DA:508:A:C3'   | 22:DA:509:C:H5'   | 2.43                     | 0.47              |
| 22:DA:681:G:C2    | 22:DA:682:G:C8    | 3.02                     | 0.47              |
| 22:DA:748:G:C8    | 40:DS:89:ALA:HB1  | 2.49                     | 0.47              |
| 22:DA:85:G:OP2    | 42:DU:7:ARG:HB2   | 2.15                     | 0.47              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 24:DC:243:HIS:O   | 24:DC:245:VAL:HG13 | 2.14                     | 0.47              |
| 26:DE:61:ARG:HD2  | 26:DE:63:LYS:O     | 2.13                     | 0.47              |
| 27:DF:128:TYR:CG  | 27:DF:170:LEU:HD13 | 2.49                     | 0.47              |
| 28:DG:98:VAL:HG22 | 28:DG:125:CYS:SG   | 2.54                     | 0.47              |
| 30:DI:59:ILE:HG22 | 30:DI:60:THR:N     | 2.29                     | 0.47              |
| 36:DO:71:ALA:HB2  | 36:DO:102:ARG:HB2  | 1.96                     | 0.47              |
| 42:DU:98:SER:O    | 42:DU:99:ASN:CB    | 2.62                     | 0.47              |
| 22:DA:400:G:N7    | 45:DX:57:ARG:NH1   | 2.62                     | 0.47              |
| 1:AA:1108:G:H2'   | 1:AA:1108:G:N3     | 2.30                     | 0.47              |
| 1:AA:1154:G:N3    | 1:AA:1154:G:H2'    | 2.28                     | 0.47              |
| 1:AA:115:G:H1'    | 1:AA:116:A:N7      | 2.30                     | 0.47              |
| 1:AA:172:A:N7     | 1:AA:174:A:N7      | 2.62                     | 0.47              |
| 1:AA:212:G:N2     | 1:AA:213:G:C4      | 2.82                     | 0.47              |
| 1:AA:939:G:H2'    | 1:AA:940:C:C6      | 2.49                     | 0.47              |
| 2:AB:91:PHE:CD2   | 2:AB:150:GLY:HA3   | 2.49                     | 0.47              |
| 10:AJ:91:ASP:OD2  | 10:AJ:91:ASP:N     | 2.47                     | 0.47              |
| 16:AP:5:ARG:HA    | 16:AP:68:SER:OG    | 2.15                     | 0.47              |
| 16:AP:61:VAL:HG22 | 16:AP:67:ILE:HD11  | 1.94                     | 0.47              |
| 53:B5:50:ILE:CB   | 53:B5:52:PRO:HD3   | 2.45                     | 0.47              |
| 22:BA:1045:C:H3'  | 22:BA:1046:A:H5'   | 1.96                     | 0.47              |
| 22:BA:1177:G:C2'  | 22:BA:1178:C:O5'   | 2.62                     | 0.47              |
| 22:BA:1171:G:N3   | 22:BA:1179:G:N1    | 2.61                     | 0.47              |
| 22:BA:1416:G:O2'  | 22:BA:1417:C:OP2   | 2.26                     | 0.47              |
| 22:BA:1866:A:N1   | 22:BA:1876:A:C8    | 2.82                     | 0.47              |
| 22:BA:2502:G:OP2  | 57:BA:3497:HOH:O   | 2.20                     | 0.47              |
| 22:BA:335:C:O2'   | 22:BA:336:C:H5'    | 2.14                     | 0.47              |
| 22:BA:481:G:C2    | 22:BA:507:A:C4     | 3.02                     | 0.47              |
| 43:BV:65:VAL:O    | 43:BV:66:ASP:C     | 2.53                     | 0.47              |
| 1:CA:1001:C:H2'   | 1:CA:1002:G:N7     | 2.29                     | 0.47              |
| 1:CA:1004:A:O2'   | 1:CA:1036:A:C2     | 2.66                     | 0.47              |
| 1:CA:1262:C:C2'   | 1:CA:1263:C:H5'    | 2.45                     | 0.47              |
| 1:CA:1479:C:C2    | 1:CA:1480:A:C8     | 3.02                     | 0.47              |
| 1:CA:106:C:O2     | 1:CA:379:C:C5'     | 2.62                     | 0.47              |
| 1:CA:414:A:H2'    | 1:CA:415:A:O4'     | 2.14                     | 0.47              |
| 1:CA:811:C:C5     | 1:CA:812:G:C6      | 3.02                     | 0.47              |
| 1:CA:859:G:H2'    | 1:CA:860:A:C8      | 2.49                     | 0.47              |
| 3:CC:42:TYR:CZ    | 3:CC:46:GLU:HG3    | 2.49                     | 0.47              |
| 5:CE:13:GLU:OE1   | 5:CE:68:ARG:NH1    | 2.45                     | 0.47              |
| 1:CA:824:G:H1'    | 8:CH:2:SER:N       | 2.29                     | 0.47              |
| 9:CI:17:ALA:HA    | 9:CI:67:VAL:HA     | 1.95                     | 0.47              |
| 12:CL:38:TYR:HB3  | 12:CL:52:VAL:HG13  | 1.95                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 14:CN:23:LYS:O     | 14:CN:26:GLU:HG3   | 2.15                     | 0.47              |
| 15:CO:13:SER:O     | 15:CO:14:GLU:HG3   | 2.14                     | 0.47              |
| 22:DA:1027:A:C5    | 22:DA:1126:A:C2    | 3.02                     | 0.47              |
| 22:DA:1043:C:C4    | 22:DA:1044:C:C4    | 3.03                     | 0.47              |
| 22:DA:1063:G:C4'   | 30:DI:77:ALA:HB1   | 2.44                     | 0.47              |
| 22:DA:1274:A:N3    | 22:DA:1297:C:H1'   | 2.30                     | 0.47              |
| 22:DA:1514:G:H5''  | 22:DA:1515:A:P     | 2.55                     | 0.47              |
| 22:DA:170:U:C2     | 22:DA:171:U:C5     | 3.02                     | 0.47              |
| 22:DA:2093:G:N7    | 22:DA:2225:A:H2'   | 2.29                     | 0.47              |
| 22:DA:2120:G:C2    | 22:DA:2121:G:C8    | 3.02                     | 0.47              |
| 22:DA:2186:G:C6    | 22:DA:2187:U:C4    | 3.02                     | 0.47              |
| 22:DA:2244:U:H2'   | 22:DA:2245:U:O4'   | 2.15                     | 0.47              |
| 22:DA:397:U:OP1    | 45:DX:31:PRO:HA    | 2.15                     | 0.47              |
| 22:DA:790:U:OP2    | 57:DA:3755:HOH:O   | 2.20                     | 0.47              |
| 26:DE:149:ILE:HG23 | 26:DE:188:MET:HA   | 1.95                     | 0.47              |
| 29:DH:117:LEU:HD11 | 29:DH:130:VAL:HG22 | 1.95                     | 0.47              |
| 29:DH:62:LEU:HD22  | 29:DH:62:LEU:O     | 2.14                     | 0.47              |
| 32:DK:99:ILE:CG2   | 32:DK:119:ALA:HB2  | 2.44                     | 0.47              |
| 38:DQ:84:LYS:O     | 38:DQ:87:SER:N     | 2.39                     | 0.47              |
| 41:DT:59:ASN:O     | 41:DT:84:TYR:N     | 2.47                     | 0.47              |
| 43:DV:38:LEU:HD23  | 43:DV:40:ILE:HD11  | 1.96                     | 0.47              |
| 1:AA:771:G:H2'     | 1:AA:772:U:H6      | 1.78                     | 0.47              |
| 1:AA:977:A:H1'     | 1:AA:982:U:O4      | 2.14                     | 0.47              |
| 2:AB:54:LEU:HD12   | 2:AB:220:THR:HG21  | 1.96                     | 0.47              |
| 2:AB:82:ASP:OD1    | 2:AB:84:ALA:HB3    | 2.13                     | 0.47              |
| 3:AC:53:SER:HB2    | 3:AC:115:LEU:HG    | 1.95                     | 0.47              |
| 4:AD:109:ALA:N     | 4:AD:113:GLU:OE2   | 2.44                     | 0.47              |
| 7:AG:97:ASN:HA     | 7:AG:100:ALA:HB3   | 1.96                     | 0.47              |
| 1:AA:1371:G:OP1    | 9:AI:13:LYS:HD3    | 2.15                     | 0.47              |
| 10:AJ:11:LYS:HA    | 10:AJ:70:HIS:O     | 2.14                     | 0.47              |
| 11:AK:76:GLU:HA    | 22:BA:2141:G:P     | 2.55                     | 0.47              |
| 1:AA:624:C:H4'     | 16:AP:11:ALA:HB2   | 1.97                     | 0.47              |
| 19:AS:42:PRO:HD3   | 19:AS:67:VAL:CG1   | 2.45                     | 0.47              |
| 20:AT:5:LYS:O      | 20:AT:7:ALA:N      | 2.47                     | 0.47              |
| 21:AU:16:LEU:HA    | 21:AU:18:ARG:CZ    | 2.43                     | 0.47              |
| 22:BA:1064:C:H4'   | 30:BI:90:SER:HB2   | 1.95                     | 0.47              |
| 22:BA:2297:A:C2    | 22:BA:2298:A:C8    | 3.02                     | 0.47              |
| 22:BA:2502:G:H5''  | 22:BA:2503:A:H5''  | 1.94                     | 0.47              |
| 22:BA:85:G:P       | 42:BU:28:VAL:HG11  | 2.54                     | 0.47              |
| 23:BB:53:A:C2      | 23:BB:54:G:C8      | 3.01                     | 0.47              |
| 24:BC:24:LEU:HD12  | 24:BC:24:LEU:HA    | 1.78                     | 0.47              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 26:BE:108:ILE:CD1 | 26:BE:180:LEU:HB3  | 2.44                     | 0.47              |
| 31:BJ:23:LYS:HE2  | 31:BJ:142:ILE:OXT  | 2.14                     | 0.47              |
| 32:BK:53:LYS:NZ   | 32:BK:56:ASP:OD2   | 2.40                     | 0.47              |
| 33:BL:77:ILE:HD11 | 33:BL:101:ILE:HG21 | 1.97                     | 0.47              |
| 39:BR:74:ILE:O    | 39:BR:86:GLN:HA    | 2.15                     | 0.47              |
| 43:BV:48:MET:SD   | 43:BV:86:LEU:CD1   | 3.02                     | 0.47              |
| 1:CA:1107:C:C2    | 1:CA:1108:G:C8     | 3.03                     | 0.47              |
| 1:CA:485:U:HO2'   | 1:CA:486:U:P       | 2.38                     | 0.47              |
| 1:CA:775:G:C2'    | 1:CA:776:G:H5'     | 2.44                     | 0.47              |
| 1:CA:951:G:N3     | 1:CA:970:C:O2'     | 2.34                     | 0.47              |
| 14:CN:67:THR:HG23 | 14:CN:83:LYS:CE    | 2.45                     | 0.47              |
| 11:CK:112:ASP:HB3 | 21:CU:4:ILE:CG2    | 2.44                     | 0.47              |
| 49:D1:39:PHE:CD2  | 49:D1:40:ASP:N     | 2.82                     | 0.47              |
| 22:DA:1115:G:O2'  | 22:DA:1116:G:OP2   | 2.25                     | 0.47              |
| 22:DA:1139:G:O2'  | 22:DA:1140:C:H5'   | 2.14                     | 0.47              |
| 22:DA:1178:C:H2'  | 22:DA:1179:G:C8    | 2.49                     | 0.47              |
| 22:DA:1204:A:C2   | 22:DA:1240:U:N3    | 2.82                     | 0.47              |
| 22:DA:1462:C:N3   | 22:DA:1463:C:C5    | 2.83                     | 0.47              |
| 22:DA:218:A:N7    | 57:DA:3226:HOH:O   | 2.36                     | 0.47              |
| 22:DA:2221:G:C2'  | 22:DA:2222:C:H5'   | 2.45                     | 0.47              |
| 22:DA:2499:C:C4   | 22:DA:2500:U:C4    | 3.02                     | 0.47              |
| 22:DA:228:C:C2    | 22:DA:418:C:H4'    | 2.50                     | 0.47              |
| 22:DA:478:A:C2    | 22:DA:480:A:C4     | 3.02                     | 0.47              |
| 22:DA:575:A:C2    | 22:DA:576:U:C6     | 3.02                     | 0.47              |
| 22:DA:979:A:C8    | 22:DA:982:C:N4     | 2.83                     | 0.47              |
| 24:DC:57:GLY:O    | 24:DC:58:HIS:O     | 2.32                     | 0.47              |
| 24:DC:67:PHE:CE2  | 24:DC:156:ARG:NH2  | 2.82                     | 0.47              |
| 26:DE:130:LYS:HB2 | 26:DE:133:LEU:CB   | 2.45                     | 0.47              |
| 34:DM:69:PRO:O    | 34:DM:93:VAL:O     | 2.33                     | 0.47              |
| 45:DX:25:THR:O    | 45:DX:25:THR:HG22  | 2.13                     | 0.47              |
| 47:DZ:41:THR:HB   | 47:DZ:42:PRO:HD2   | 1.95                     | 0.47              |
| 1:AA:1130:A:N3    | 1:AA:1146:A:C4     | 2.82                     | 0.47              |
| 1:AA:1203:C:C2    | 1:AA:1204:A:C8     | 3.02                     | 0.47              |
| 1:AA:408:A:C2     | 1:AA:435:A:C2      | 3.03                     | 0.47              |
| 1:AA:654:G:C2'    | 1:AA:655:A:H5'     | 2.45                     | 0.47              |
| 1:AA:741:G:H2'    | 1:AA:742:G:O4'     | 2.15                     | 0.47              |
| 1:AA:880:C:C2'    | 1:AA:881:G:H5'     | 2.44                     | 0.47              |
| 2:AB:166:ALA:HB2  | 2:AB:187:VAL:HG12  | 1.96                     | 0.47              |
| 2:AB:64:LYS:HA    | 2:AB:64:LYS:HE2    | 1.95                     | 0.47              |
| 4:AD:130:VAL:CG1  | 4:AD:135:TYR:CD1   | 2.98                     | 0.47              |
| 7:AG:145:ALA:O    | 7:AG:146:GLU:HB3   | 2.15                     | 0.47              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 9:AI:23:PRO:HA     | 9:AI:61:LEU:HA    | 1.95                     | 0.47              |
| 9:AI:44:ALA:H      | 9:AI:46:MET:HE1   | 1.80                     | 0.47              |
| 1:AA:1216:A:OP1    | 14:AN:3:LYS:HE2   | 2.15                     | 0.47              |
| 1:AA:667:G:H4'     | 15:AO:51:HIS:CE1  | 2.50                     | 0.47              |
| 17:AQ:61:ILE:HG22  | 17:AQ:73:TRP:CE3  | 2.50                     | 0.47              |
| 49:B1:39:PHE:HB2   | 49:B1:46:HIS:CE1  | 2.49                     | 0.47              |
| 22:BA:1072:C:C2    | 22:BA:1093:G:O6   | 2.68                     | 0.47              |
| 22:BA:1171:G:C6    | 22:BA:1172:C:N3   | 2.82                     | 0.47              |
| 22:BA:1392:A:C6    | 22:BA:1393:A:C6   | 3.02                     | 0.47              |
| 22:BA:1789:A:H5''  | 24:BC:219:THR:O   | 2.14                     | 0.47              |
| 22:BA:2038:G:H2'   | 22:BA:2039:U:O4'  | 2.13                     | 0.47              |
| 22:BA:2495:G:H2'   | 22:BA:2496:C:H5'  | 1.96                     | 0.47              |
| 22:BA:368:A:N6     | 22:BA:369:U:O4    | 2.48                     | 0.47              |
| 22:BA:684:G:C6     | 22:BA:774:G:C4    | 3.03                     | 0.47              |
| 28:BG:101:ASN:CG   | 28:BG:101:ASN:O   | 2.53                     | 0.47              |
| 28:BG:83:PHE:CE2   | 28:BG:138:LYS:HB2 | 2.49                     | 0.47              |
| 29:BH:111:ALA:O    | 29:BH:114:GLU:HB2 | 2.13                     | 0.47              |
| 29:BH:117:LEU:HD23 | 29:BH:121:VAL:HA  | 1.95                     | 0.47              |
| 23:BB:91:C:OP2     | 34:BM:18:ARG:NH2  | 2.46                     | 0.47              |
| 39:BR:102:SER:O    | 39:BR:103:ALA:O   | 2.33                     | 0.47              |
| 42:BU:98:SER:C     | 42:BU:100:SER:H   | 2.18                     | 0.47              |
| 1:CA:1343:G:O2'    | 9:CI:123:ARG:HD2  | 2.15                     | 0.47              |
| 1:CA:976:G:H1'     | 1:CA:1363:A:N6    | 2.30                     | 0.47              |
| 1:CA:302:G:O2'     | 1:CA:556:C:H5''   | 2.15                     | 0.47              |
| 1:CA:330:C:O2      | 1:CA:330:C:H2'    | 2.13                     | 0.47              |
| 1:CA:350:G:C6      | 1:CA:351:G:O6     | 2.67                     | 0.47              |
| 1:CA:375:U:N3      | 1:CA:376:G:N7     | 2.63                     | 0.47              |
| 1:CA:651:C:N4      | 1:CA:652:U:O4     | 2.47                     | 0.47              |
| 1:CA:771:G:C2      | 1:CA:809:G:C2     | 3.03                     | 0.47              |
| 2:CB:71:GLY:HA2    | 2:CB:164:ILE:CG2  | 2.45                     | 0.47              |
| 2:CB:186:ILE:HG13  | 2:CB:200:ILE:O    | 2.15                     | 0.47              |
| 5:CE:16:ILE:CD1    | 5:CE:38:VAL:HG23  | 2.44                     | 0.47              |
| 3:CC:168:TYR:OH    | 5:CE:55:GLU:OE1   | 2.31                     | 0.47              |
| 9:CI:101:ALA:HB1   | 9:CI:103:PHE:CZ   | 2.50                     | 0.47              |
| 10:CJ:7:ARG:HD2    | 10:CJ:73:LEU:HD21 | 1.97                     | 0.47              |
| 12:CL:3:THR:O      | 12:CL:4:VAL:C     | 2.53                     | 0.47              |
| 20:CT:67:ILE:CD1   | 20:CT:71:LYS:HE3  | 2.44                     | 0.47              |
| 22:DA:1409:U:H2'   | 22:DA:1410:G:O4'  | 2.14                     | 0.47              |
| 22:DA:1649:G:C6    | 22:DA:2009:A:N6   | 2.82                     | 0.47              |
| 22:DA:1855:U:C4    | 22:DA:1856:U:C4   | 3.03                     | 0.47              |
| 22:DA:241:A:N1     | 22:DA:255:A:H5''  | 2.29                     | 0.47              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 22:DA:2586:U:H2'   | 22:DA:2587:A:O4'  | 2.14                     | 0.47              |
| 22:DA:288:U:H2'    | 22:DA:289:G:O4'   | 2.14                     | 0.47              |
| 22:DA:537:G:C6     | 22:DA:555:G:C2    | 3.02                     | 0.47              |
| 22:DA:591:U:C2     | 22:DA:592:A:C8    | 3.03                     | 0.47              |
| 22:DA:658:U:C2     | 22:DA:659:G:C8    | 3.02                     | 0.47              |
| 22:DA:945:A:N7     | 22:DA:2448:A:C2   | 2.83                     | 0.47              |
| 23:DB:109:A:C5     | 23:DB:110:C:C4    | 3.02                     | 0.47              |
| 22:DA:1245:G:H4'   | 26:DE:33:VAL:CG1  | 2.44                     | 0.47              |
| 33:DL:116:VAL:HG21 | 33:DL:134:ALA:C   | 2.35                     | 0.47              |
| 36:DO:58:ILE:O     | 36:DO:58:ILE:HG22 | 2.14                     | 0.47              |
| 1:AA:1269:A:N1     | 1:AA:1313:U:O4'   | 2.48                     | 0.47              |
| 1:AA:507:C:C4      | 1:AA:508:U:C4     | 3.03                     | 0.47              |
| 1:AA:520:A:N1      | 1:AA:536:C:H1'    | 2.30                     | 0.47              |
| 1:AA:820:U:H4'     | 1:AA:821:G:OP2    | 2.14                     | 0.47              |
| 2:AB:216:ALA:O     | 2:AB:219:ALA:O    | 2.33                     | 0.47              |
| 5:AE:98:PRO:O      | 5:AE:99:ALA:HB3   | 2.14                     | 0.47              |
| 7:AG:129:GLU:O     | 7:AG:130:ASN:C    | 2.53                     | 0.47              |
| 7:AG:68:ASN:O      | 7:AG:138:ARG:HD3  | 2.15                     | 0.47              |
| 11:AK:128:ARG:HH11 | 11:AK:128:ARG:HG2 | 1.79                     | 0.47              |
| 15:AO:81:LEU:HD12  | 15:AO:85:LEU:CD2  | 2.44                     | 0.47              |
| 19:AS:63:THR:O     | 19:AS:65:GLU:N    | 2.47                     | 0.47              |
| 21:AU:11:PRO:O     | 21:AU:12:PHE:CB   | 2.63                     | 0.47              |
| 22:BA:1059:G:O2'   | 30:BI:129:ILE:HA  | 2.14                     | 0.47              |
| 22:BA:1106:G:N3    | 22:BA:1106:G:H2'  | 2.29                     | 0.47              |
| 22:BA:1107:G:C4    | 22:BA:1108:U:C6   | 3.03                     | 0.47              |
| 22:BA:811:U:C2     | 22:BA:1251:C:C5   | 3.02                     | 0.47              |
| 22:BA:1386:C:H2'   | 22:BA:1387:A:C8   | 2.49                     | 0.47              |
| 22:BA:1914:C:H2'   | 22:BA:1914:C:O2   | 2.14                     | 0.47              |
| 22:BA:2213:U:H4'   | 22:BA:2214:C:OP2  | 2.15                     | 0.47              |
| 22:BA:547:A:H3'    | 22:BA:548:G:C5'   | 2.44                     | 0.47              |
| 22:BA:618:G:C6     | 22:BA:619:G:C4    | 3.03                     | 0.47              |
| 22:BA:997:G:O2'    | 22:BA:998:C:H5'   | 2.15                     | 0.47              |
| 22:BA:801:G:C4     | 26:BE:49:ARG:HD3  | 2.50                     | 0.47              |
| 27:BF:5:HIS:O      | 27:BF:8:TYR:HB3   | 2.15                     | 0.47              |
| 30:BI:108:GLU:HA   | 30:BI:111:GLN:HB3 | 1.96                     | 0.47              |
| 32:BK:91:SER:O     | 32:BK:92:GLU:C    | 2.53                     | 0.47              |
| 33:BL:94:THR:HG22  | 33:BL:95:LEU:N    | 2.29                     | 0.47              |
| 39:BR:64:VAL:HG23  | 39:BR:65:ALA:N    | 2.29                     | 0.47              |
| 41:BT:18:GLU:N     | 41:BT:18:GLU:CD   | 2.68                     | 0.47              |
| 1:CA:1272:G:H2'    | 1:CA:1273:C:O4'   | 2.15                     | 0.47              |
| 1:CA:211:G:O2'     | 1:CA:212:G:H4'    | 2.15                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CA:455:G:C6     | 1:CA:456:A:C6     | 3.03                     | 0.47              |
| 1:CA:484:G:C5     | 1:CA:486:U:H1'    | 2.49                     | 0.47              |
| 1:CA:784:A:H2'    | 1:CA:785:G:C8     | 2.50                     | 0.47              |
| 2:CB:187:VAL:HG23 | 2:CB:188:ASP:O    | 2.14                     | 0.47              |
| 2:CB:68:LEU:HD22  | 2:CB:70:VAL:HG23  | 1.94                     | 0.47              |
| 5:CE:105:ILE:HG13 | 5:CE:105:ILE:O    | 2.14                     | 0.47              |
| 7:CG:42:ILE:O     | 7:CG:42:ILE:CG2   | 2.63                     | 0.47              |
| 5:CE:83:HIS:CD2   | 8:CH:96:MET:HE2   | 2.50                     | 0.47              |
| 10:CJ:15:HIS:HB3  | 10:CJ:70:HIS:NE2  | 2.29                     | 0.47              |
| 10:CJ:15:HIS:HB3  | 10:CJ:70:HIS:CD2  | 2.50                     | 0.47              |
| 11:CK:50:SER:HB3  | 11:CK:65:VAL:CG2  | 2.45                     | 0.47              |
| 12:CL:59:ASN:N    | 12:CL:59:ASN:HD22 | 2.13                     | 0.47              |
| 14:CN:3:LYS:HD3   | 14:CN:6:MET:HG2   | 1.97                     | 0.47              |
| 20:CT:67:ILE:O    | 20:CT:68:HIS:C    | 2.52                     | 0.47              |
| 22:DA:1248:G:C5   | 26:DE:46:GLN:NE2  | 2.83                     | 0.47              |
| 22:DA:1310:G:H2'  | 22:DA:1311:G:H5'  | 1.95                     | 0.47              |
| 22:DA:1428:C:C5   | 22:DA:1569:A:H5'' | 2.50                     | 0.47              |
| 22:DA:1577:C:H2'  | 22:DA:1578:U:C1'  | 2.45                     | 0.47              |
| 22:DA:2199:A:N7   | 22:DA:2225:A:C6   | 2.83                     | 0.47              |
| 22:DA:2199:A:N7   | 22:DA:2225:A:N6   | 2.63                     | 0.47              |
| 22:DA:2385:C:H2'  | 22:DA:2386:A:C8   | 2.49                     | 0.47              |
| 22:DA:2531:A:C4   | 22:DA:2532:G:C8   | 3.02                     | 0.47              |
| 22:DA:260:G:C6    | 22:DA:261:G:N7    | 2.82                     | 0.47              |
| 22:DA:2822:G:H2'  | 22:DA:2823:A:H5'' | 1.97                     | 0.47              |
| 22:DA:396:G:H2'   | 22:DA:397:U:O5'   | 2.15                     | 0.47              |
| 22:DA:39:G:C5     | 22:DA:40:U:C5     | 3.01                     | 0.47              |
| 22:DA:46:G:N1     | 22:DA:47:C:C4     | 2.83                     | 0.47              |
| 23:DB:109:A:C6    | 23:DB:110:C:N3    | 2.82                     | 0.47              |
| 24:DC:125:LYS:O   | 24:DC:192:LEU:HB2 | 2.15                     | 0.47              |
| 26:DE:8:ALA:O     | 26:DE:9:GLN:HB2   | 2.15                     | 0.47              |
| 27:DF:72:LYS:HG3  | 27:DF:74:VAL:HG13 | 1.96                     | 0.47              |
| 28:DG:158:LYS:O   | 28:DG:159:GLY:C   | 2.52                     | 0.47              |
| 33:DL:82:LEU:O    | 33:DL:82:LEU:HG   | 2.15                     | 0.47              |
| 43:DV:48:MET:SD   | 43:DV:86:LEU:HG   | 2.54                     | 0.47              |
| 43:DV:9:ARG:NH2   | 43:DV:17:SER:OG   | 2.48                     | 0.47              |
| 22:DA:371:A:N3    | 45:DX:61:LYS:NZ   | 2.62                     | 0.47              |
| 1:AA:200:G:N2     | 1:AA:218:U:C2     | 2.82                     | 0.47              |
| 1:AA:261:U:P      | 20:AT:71:LYS:HE2  | 2.55                     | 0.47              |
| 1:AA:443:C:O2'    | 1:AA:444:G:H5'    | 2.15                     | 0.47              |
| 1:AA:667:G:OP1    | 1:AA:732:C:O2'    | 2.26                     | 0.47              |
| 1:AA:803:G:C5     | 1:AA:804:U:C4     | 3.02                     | 0.47              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:AA:872:A:C4     | 1:AA:874:G:C8    | 3.03                     | 0.47              |
| 4:AD:32:CYS:SG    | 4:AD:33:LYS:N    | 2.88                     | 0.47              |
| 6:AF:29:ILE:HG23  | 6:AF:66:ALA:HB2  | 1.97                     | 0.47              |
| 6:AF:3:HIS:CE1    | 6:AF:65:GLU:OE2  | 2.67                     | 0.47              |
| 6:AF:91:ARG:HG2   | 6:AF:93:LYS:CE   | 2.44                     | 0.47              |
| 8:AH:80:ARG:HB2   | 8:AH:81:PRO:HD2  | 1.96                     | 0.47              |
| 9:AI:36:GLU:HA    | 9:AI:40:GLY:HA3  | 1.96                     | 0.47              |
| 14:AN:73:PHE:CD1  | 14:AN:74:LEU:N   | 2.83                     | 0.47              |
| 22:BA:819:A:C4    | 22:BA:1189:A:C2  | 3.03                     | 0.47              |
| 22:BA:120:U:H5'   | 22:BA:122:G:OP2  | 2.14                     | 0.47              |
| 22:BA:181:A:C2    | 22:BA:182:A:C4   | 3.02                     | 0.47              |
| 22:BA:211:C:O2'   | 22:BA:212:G:H5'  | 2.14                     | 0.47              |
| 22:BA:2492:U:H2'  | 22:BA:2493:U:H6  | 1.80                     | 0.47              |
| 22:BA:2593:U:H2'  | 22:BA:2594:C:O5' | 2.14                     | 0.47              |
| 26:BE:149:ILE:CD1 | 26:BE:172:ALA:HA | 2.45                     | 0.47              |
| 30:BI:39:CYS:HA   | 30:BI:42:PHE:HB2 | 1.96                     | 0.47              |
| 37:BP:37:LYS:HD3  | 37:BP:39:ARG:NH1 | 2.30                     | 0.47              |
| 47:BZ:24:LEU:HD11 | 47:BZ:54:MET:HE1 | 1.97                     | 0.47              |
| 1:CA:1014:A:N7    | 1:CA:1015:G:C6   | 2.82                     | 0.47              |
| 1:CA:1129:C:C6    | 1:CA:1139:G:C8   | 3.02                     | 0.47              |
| 1:CA:939:G:C6     | 1:CA:940:C:C4    | 3.03                     | 0.47              |
| 2:CB:57:LEU:HD11  | 2:CB:221:VAL:CG2 | 2.45                     | 0.47              |
| 3:CC:71:ALA:HA    | 3:CC:106:VAL:HB  | 1.96                     | 0.47              |
| 4:CD:174:ASP:O    | 4:CD:175:ALA:HB2 | 2.14                     | 0.47              |
| 9:CI:26:GLY:N     | 9:CI:61:LEU:O    | 2.47                     | 0.47              |
| 10:CJ:57:VAL:HG22 | 10:CJ:58:ASN:H   | 1.79                     | 0.47              |
| 22:DA:1357:C:N4   | 22:DA:1358:G:C6  | 2.83                     | 0.47              |
| 22:DA:143:C:H2'   | 22:DA:144:A:H5'  | 1.96                     | 0.47              |
| 22:DA:1596:A:C6   | 22:DA:1597:A:C6  | 3.03                     | 0.47              |
| 22:DA:1343:G:H4'  | 22:DA:1598:A:OP2 | 2.15                     | 0.47              |
| 22:DA:1776:G:N2   | 22:DA:1789:A:H1' | 2.30                     | 0.47              |
| 22:DA:1791:A:C2'  | 22:DA:1792:G:H5' | 2.45                     | 0.47              |
| 22:DA:1797:G:O3'  | 24:DC:256:LYS:HA | 2.15                     | 0.47              |
| 22:DA:1835:G:C4   | 22:DA:1836:C:C6  | 3.02                     | 0.47              |
| 22:DA:1652:A:C2   | 22:DA:2006:C:N3  | 2.82                     | 0.47              |
| 22:DA:2054:A:OP1  | 22:DA:2055:C:O2' | 2.29                     | 0.47              |
| 22:DA:2115:G:H2'  | 22:DA:2117:A:N7  | 2.30                     | 0.47              |
| 22:DA:965:C:H4'   | 22:DA:2273:A:H1' | 1.96                     | 0.47              |
| 22:DA:2449:U:H4'  | 22:DA:2450:A:OP1 | 2.15                     | 0.47              |
| 22:DA:248:G:H5'   | 22:DA:250:G:N7   | 2.28                     | 0.47              |
| 22:DA:2511:U:C5   | 22:DA:2512:C:C5  | 3.03                     | 0.47              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:DA:2796:U:N3   | 22:DA:2798:U:C4    | 2.83                     | 0.47              |
| 22:DA:2829:A:H2'  | 22:DA:2830:C:H5'   | 1.96                     | 0.47              |
| 22:DA:526:A:P     | 57:DA:3247:HOH:O   | 2.72                     | 0.47              |
| 22:DA:892:A:N3    | 22:DA:892:A:H3'    | 2.30                     | 0.47              |
| 25:DD:35:THR:O    | 25:DD:36:GLN:HB2   | 2.14                     | 0.47              |
| 26:DE:106:LYS:HG3 | 26:DE:200:LEU:HD23 | 1.95                     | 0.47              |
| 30:DI:56:PRO:HD2  | 30:DI:75:PRO:HD3   | 1.97                     | 0.47              |
| 32:DK:108:ARG:HB2 | 32:DK:116:ILE:HD13 | 1.95                     | 0.47              |
| 36:DO:104:GLN:O   | 36:DO:107:ALA:N    | 2.47                     | 0.47              |
| 36:DO:117:PHE:CD1 | 36:DO:117:PHE:C    | 2.88                     | 0.47              |
| 40:DS:55:ILE:CG2  | 40:DS:66:ILE:CD1   | 2.93                     | 0.47              |
| 41:DT:27:SER:O    | 41:DT:29:THR:N     | 2.48                     | 0.47              |
| 41:DT:7:LEU:HD22  | 41:DT:46:ALA:CA    | 2.45                     | 0.47              |
| 45:DX:12:PRO:HB3  | 45:DX:28:ARG:NH2   | 2.29                     | 0.47              |
| 45:DX:56:MET:O    | 45:DX:60:ASP:N     | 2.44                     | 0.47              |
| 1:AA:1126:U:O2    | 1:AA:1280:A:H5'    | 2.15                     | 0.47              |
| 1:AA:1330:U:C4    | 1:AA:1331:G:C6     | 3.03                     | 0.47              |
| 1:AA:1493:A:O2'   | 1:AA:1494:G:P      | 2.73                     | 0.47              |
| 1:AA:469:C:C5     | 1:AA:470:C:C4      | 3.03                     | 0.47              |
| 1:AA:568:G:C4     | 1:AA:569:C:H5      | 2.31                     | 0.47              |
| 2:AB:12:ALA:HB1   | 2:AB:15:HIS:HB3    | 1.97                     | 0.47              |
| 2:AB:94:HIS:O     | 2:AB:95:ARG:C      | 2.52                     | 0.47              |
| 3:AC:112:ASP:O    | 3:AC:116:VAL:HG23  | 2.14                     | 0.47              |
| 10:AJ:17:LEU:HD21 | 10:AJ:96:VAL:HG22  | 1.97                     | 0.47              |
| 10:AJ:36:VAL:HG22 | 10:AJ:76:ILE:HG12  | 1.97                     | 0.47              |
| 13:AM:91:HIS:CE1  | 13:AM:97:VAL:HG21  | 2.49                     | 0.47              |
| 15:AO:70:LEU:HD21 | 15:AO:77:ARG:HB2   | 1.97                     | 0.47              |
| 21:AU:10:GLU:CB   | 21:AU:11:PRO:HD3   | 2.45                     | 0.47              |
| 51:B3:26:HIS:HB2  | 51:B3:44:LEU:O     | 2.15                     | 0.47              |
| 52:B4:25:VAL:HB   | 52:B4:35:GLN:HB2   | 1.96                     | 0.47              |
| 53:B5:28:ARG:O    | 53:B5:28:ARG:CG    | 2.63                     | 0.47              |
| 22:BA:1696:G:O6   | 22:BA:1697:G:C2    | 2.68                     | 0.47              |
| 22:BA:204:A:O4'   | 22:BA:206:U:C6     | 2.67                     | 0.47              |
| 22:BA:2076:U:O4'  | 22:BA:2076:U:O2    | 2.30                     | 0.47              |
| 22:BA:2469:A:C2   | 22:BA:2482:A:C4    | 3.01                     | 0.47              |
| 22:BA:2756:U:H1'  | 22:BA:2757:A:H5''  | 1.97                     | 0.47              |
| 22:BA:279:A:N6    | 22:BA:361:G:O2'    | 2.46                     | 0.47              |
| 22:BA:569:U:H1'   | 22:BA:947:A:O4'    | 2.14                     | 0.47              |
| 22:BA:748:G:C8    | 40:BS:89:ALA:HB1   | 2.49                     | 0.47              |
| 22:BA:975:A:C2    | 22:BA:990:A:C8     | 3.03                     | 0.47              |
| 25:BD:85:ALA:O    | 25:BD:86:GLU:C     | 2.53                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 26:BE:37:ALA:O    | 26:BE:40:ARG:HB2  | 2.14                     | 0.47              |
| 27:BF:121:SER:HB3 | 27:BF:129:SER:O   | 2.15                     | 0.47              |
| 29:BH:14:SER:O    | 29:BH:15:LEU:CB   | 2.61                     | 0.47              |
| 29:BH:97:ARG:HH11 | 1:CA:370:C:C5'    | 2.28                     | 0.47              |
| 30:BI:6:GLN:O     | 30:BI:7:ALA:HB3   | 2.15                     | 0.47              |
| 31:BJ:17:VAL:HG23 | 31:BJ:137:PRO:CB  | 2.45                     | 0.47              |
| 22:BA:2839:G:H4'  | 35:BN:49:GLU:OE1  | 2.15                     | 0.47              |
| 40:BS:46:LEU:O    | 40:BS:50:VAL:HG23 | 2.15                     | 0.47              |
| 1:CA:1152:A:H4'   | 10:CJ:15:HIS:CD2  | 2.50                     | 0.47              |
| 1:CA:1299:A:N3    | 1:CA:1299:A:H2'   | 2.30                     | 0.47              |
| 1:CA:421:U:O5'    | 1:CA:422:C:H5     | 1.96                     | 0.47              |
| 1:CA:505:G:C6     | 1:CA:535:A:C2     | 3.03                     | 0.47              |
| 1:CA:642:A:H2'    | 1:CA:643:C:C6     | 2.50                     | 0.47              |
| 1:CA:991:U:H4'    | 1:CA:992:U:H5''   | 1.96                     | 0.47              |
| 5:CE:111:MET:HG3  | 5:CE:140:THR:HG21 | 1.96                     | 0.47              |
| 7:CG:66:LEU:HG    | 7:CG:66:LEU:O     | 2.15                     | 0.47              |
| 17:CQ:14:SER:CB   | 17:CQ:22:VAL:HG12 | 2.45                     | 0.47              |
| 19:CS:6:LYS:HB2   | 19:CS:7:LYS:HE2   | 1.95                     | 0.47              |
| 22:DA:1563:U:H2'  | 22:DA:1564:C:C6   | 2.49                     | 0.47              |
| 22:DA:1724:G:O6   | 22:DA:1736:U:C2   | 2.68                     | 0.47              |
| 22:DA:1730:C:O2'  | 22:DA:1731:G:C2   | 2.67                     | 0.47              |
| 22:DA:195:A:C6    | 22:DA:198:C:C5    | 3.03                     | 0.47              |
| 22:DA:2121:G:C2   | 22:DA:2177:C:O2   | 2.68                     | 0.47              |
| 22:DA:2387:U:H1'  | 44:DW:41:ARG:HD2  | 1.97                     | 0.47              |
| 22:DA:2415:G:C2   | 22:DA:2416:C:C2   | 3.03                     | 0.47              |
| 22:DA:2603:G:C6   | 22:DA:2604:U:C5   | 3.02                     | 0.47              |
| 22:DA:2752:C:C5   | 22:DA:2753:A:N7   | 2.82                     | 0.47              |
| 22:DA:408:G:C6    | 22:DA:409:G:C5    | 3.03                     | 0.47              |
| 22:DA:453:A:H4'   | 22:DA:472:A:H62   | 1.78                     | 0.47              |
| 25:DD:13:ARG:HD3  | 25:DD:21:SER:OG   | 2.14                     | 0.47              |
| 25:DD:3:GLY:O     | 25:DD:82:PHE:CE1  | 2.68                     | 0.47              |
| 28:DG:83:PHE:CD2  | 28:DG:138:LYS:HB2 | 2.50                     | 0.47              |
| 29:DH:5:LEU:HD13  | 29:DH:13:GLY:HA3  | 1.96                     | 0.47              |
| 31:DJ:19:ASP:O    | 31:DJ:23:LYS:CE   | 2.63                     | 0.47              |
| 40:DS:55:ILE:HG21 | 40:DS:66:ILE:CD1  | 2.44                     | 0.47              |
| 1:AA:1049:U:O4'   | 1:AA:1201:A:C8    | 2.67                     | 0.47              |
| 1:AA:192:A:C6     | 1:AA:193:C:C4     | 3.03                     | 0.47              |
| 1:AA:642:A:N7     | 8:AH:107:SER:HA   | 2.29                     | 0.47              |
| 1:AA:689:C:O2'    | 1:AA:705:G:O2'    | 2.24                     | 0.47              |
| 1:AA:901:A:C5     | 1:AA:902:G:H1'    | 2.50                     | 0.47              |
| 2:AB:106:THR:O    | 2:AB:107:VAL:HG23 | 2.14                     | 0.47              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:AC:174:PRO:C    | 3:AC:176:HIS:H    | 2.18                     | 0.47              |
| 6:AF:63:ASN:OD1   | 6:AF:96:VAL:HG21  | 2.13                     | 0.47              |
| 10:AJ:6:ILE:CD1   | 10:AJ:76:ILE:HB   | 2.45                     | 0.47              |
| 14:AN:43:ASN:C    | 14:AN:45:VAL:H    | 2.17                     | 0.47              |
| 1:AA:263:A:P      | 20:AT:74:ARG:NH1  | 2.88                     | 0.47              |
| 53:B5:52:PRO:O    | 53:B5:53:ARG:HB2  | 2.15                     | 0.47              |
| 22:BA:1006:C:P    | 57:BA:3780:HOH:O  | 2.72                     | 0.47              |
| 22:BA:1107:G:C5   | 22:BA:1108:U:C5   | 3.03                     | 0.47              |
| 22:BA:1503:A:N6   | 22:BA:1504:A:N6   | 2.63                     | 0.47              |
| 22:BA:1730:C:O2'  | 22:BA:1731:G:C4   | 2.60                     | 0.47              |
| 22:BA:2304:G:H4'  | 27:BF:129:SER:O   | 2.14                     | 0.47              |
| 22:BA:26:G:C2'    | 22:BA:27:G:O5'    | 2.63                     | 0.47              |
| 22:BA:2681:C:C2   | 22:BA:2724:U:O4   | 2.68                     | 0.47              |
| 25:BD:125:TRP:CE3 | 25:BD:160:LYS:HD2 | 2.49                     | 0.47              |
| 36:BO:49:VAL:HG13 | 36:BO:50:ALA:N    | 2.30                     | 0.47              |
| 41:BT:2:ILE:HG12  | 41:BT:7:LEU:HD11  | 1.97                     | 0.47              |
| 1:CA:1410:A:H2'   | 1:CA:1411:C:C6    | 2.50                     | 0.47              |
| 1:CA:1486:G:H2'   | 1:CA:1487:G:O4'   | 2.14                     | 0.47              |
| 29:BH:97:ARG:NH1  | 1:CA:370:C:C5'    | 2.77                     | 0.47              |
| 1:CA:570:G:H2'    | 1:CA:570:G:N3     | 2.28                     | 0.47              |
| 5:CE:56:VAL:N     | 5:CE:57:PRO:CD    | 2.77                     | 0.47              |
| 13:CM:86:TYR:O    | 13:CM:90:ARG:CG   | 2.63                     | 0.47              |
| 16:CP:19:VAL:CG1  | 16:CP:37:GLY:N    | 2.78                     | 0.47              |
| 21:CU:32:VAL:HG12 | 21:CU:32:VAL:O    | 2.15                     | 0.47              |
| 22:DA:104:A:C5    | 22:DA:105:C:N3    | 2.83                     | 0.47              |
| 22:DA:504:A:C2    | 22:DA:1234:U:H4'  | 2.50                     | 0.47              |
| 22:DA:1308:A:N6   | 22:DA:1309:G:C2   | 2.83                     | 0.47              |
| 22:DA:1357:C:O2'  | 22:DA:1358:G:H5'  | 2.15                     | 0.47              |
| 22:DA:1588:G:C5   | 22:DA:1589:U:C4   | 3.02                     | 0.47              |
| 22:DA:178:G:C5    | 22:DA:179:C:C5    | 3.03                     | 0.47              |
| 22:DA:1965:C:H3'  | 22:DA:1966:A:H8   | 1.80                     | 0.47              |
| 22:DA:2111:U:O2   | 22:DA:2111:U:O4'  | 2.32                     | 0.47              |
| 22:DA:2282:G:N3   | 22:DA:2425:A:N6   | 2.63                     | 0.47              |
| 23:DB:60:C:N4     | 57:DB:303:HOH:O   | 2.47                     | 0.47              |
| 26:DE:47:LYS:O    | 26:DE:83:VAL:CB   | 2.63                     | 0.47              |
| 30:DI:54:PRO:HB2  | 30:DI:78:VAL:HG21 | 1.97                     | 0.47              |
| 30:DI:10:LYS:HB2  | 30:DI:56:PRO:HB3  | 1.96                     | 0.47              |
| 40:DS:41:LYS:O    | 40:DS:42:LYS:C    | 2.51                     | 0.47              |
| 42:DU:74:ASN:ND2  | 42:DU:96:PHE:CD1  | 2.82                     | 0.47              |
| 1:AA:1053:G:N2    | 1:AA:1056:U:C5    | 2.83                     | 0.47              |
| 1:AA:104:G:N2     | 1:AA:105:G:C4     | 2.82                     | 0.47              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:AA:1402:C:H2'    | 1:AA:1403:C:O4'   | 2.15                     | 0.47              |
| 1:AA:237:G:OP1     | 17:AQ:42:THR:OG1  | 2.33                     | 0.47              |
| 1:AA:704:A:C6      | 1:AA:705:G:C5     | 3.02                     | 0.47              |
| 5:AE:35:ALA:CB     | 5:AE:60:ILE:HA    | 2.45                     | 0.47              |
| 9:AI:36:GLU:HA     | 9:AI:40:GLY:CA    | 2.45                     | 0.47              |
| 19:AS:29:LYS:HB3   | 19:AS:30:PRO:HD2  | 1.97                     | 0.47              |
| 19:AS:42:PRO:O     | 19:AS:45:ILE:HG13 | 2.15                     | 0.47              |
| 53:B5:50:ILE:C     | 53:B5:52:PRO:CD   | 2.82                     | 0.47              |
| 22:BA:1178:C:H2'   | 22:BA:1179:G:C8   | 2.50                     | 0.47              |
| 22:BA:2297:A:C2    | 22:BA:2321:U:H5   | 2.33                     | 0.47              |
| 22:BA:322:A:C6     | 22:BA:340:A:N1    | 2.83                     | 0.47              |
| 22:BA:508:A:H4'    | 22:BA:509:C:OP2   | 2.15                     | 0.47              |
| 22:BA:744:U:OP1    | 57:BA:3655:HOH:O  | 2.20                     | 0.47              |
| 22:BA:954:G:C5     | 22:BA:955:U:C5    | 3.02                     | 0.47              |
| 23:BB:104:A:H2'    | 23:BB:105:G:O4'   | 2.14                     | 0.47              |
| 24:BC:162:VAL:CG1  | 24:BC:174:LEU:HB3 | 2.45                     | 0.47              |
| 25:BD:172:VAL:HG21 | 25:BD:194:PRO:HD3 | 1.96                     | 0.47              |
| 27:BF:152:LEU:HD12 | 27:BF:153:ASP:N   | 2.29                     | 0.47              |
| 28:BG:111:HIS:CD2  | 28:BG:112:PRO:O   | 2.68                     | 0.47              |
| 31:BJ:81:ILE:HG12  | 31:BJ:82:GLY:H    | 1.80                     | 0.47              |
| 35:BN:106:ASP:C    | 35:BN:106:ASP:OD1 | 2.52                     | 0.47              |
| 35:BN:32:GLU:OE1   | 35:BN:86:ARG:NH2  | 2.41                     | 0.47              |
| 36:BO:31:THR:HG23  | 36:BO:32:PRO:N    | 2.30                     | 0.47              |
| 22:BA:1250:G:C5'   | 38:BQ:6:ARG:HD3   | 2.45                     | 0.47              |
| 39:BR:21:ARG:NE    | 39:BR:93:PHE:CD1  | 2.83                     | 0.47              |
| 44:BW:51:VAL:HG13  | 44:BW:60:PHE:O    | 2.15                     | 0.47              |
| 1:CA:1034:G:H5'    | 1:CA:1035:A:OP2   | 2.15                     | 0.47              |
| 1:CA:1092:A:N1     | 1:CA:1183:U:O2    | 2.48                     | 0.47              |
| 1:CA:1381:U:O2'    | 1:CA:1382:C:O5'   | 2.33                     | 0.47              |
| 1:CA:162:A:H2'     | 1:CA:163:C:O4'    | 2.15                     | 0.47              |
| 1:CA:459:A:C8      | 1:CA:459:A:OP2    | 2.68                     | 0.47              |
| 1:CA:846:G:C2      | 1:CA:847:G:C8     | 3.03                     | 0.47              |
| 10:CJ:19:ASP:HA    | 10:CJ:22:THR:HB   | 1.97                     | 0.47              |
| 10:CJ:41:PRO:O     | 10:CJ:42:LEU:HB2  | 2.14                     | 0.47              |
| 13:CM:37:ALA:CB    | 13:CM:56:LEU:HG   | 2.44                     | 0.47              |
| 3:CC:30:ALA:HB1    | 14:CN:65:ARG:NH2  | 2.30                     | 0.47              |
| 22:DA:116:C:O2'    | 22:DA:126:A:C2'   | 2.62                     | 0.47              |
| 22:DA:1264:A:C8    | 22:DA:1265:A:C8   | 3.03                     | 0.47              |
| 22:DA:1431:A:C6    | 22:DA:1432:G:C5   | 3.03                     | 0.47              |
| 22:DA:152:A:C2     | 22:DA:175:G:N3    | 2.82                     | 0.47              |
| 22:DA:160:A:N6     | 22:DA:161:A:N6    | 2.63                     | 0.47              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 22:DA:1805:A:C2     | 22:DA:1813:G:C6    | 3.03                     | 0.47              |
| 22:DA:187:G:N1      | 22:DA:210:C:C2     | 2.82                     | 0.47              |
| 22:DA:1896:G:H2'    | 22:DA:1897:G:O4'   | 2.15                     | 0.47              |
| 22:DA:2403:C:H2'    | 22:DA:2403:C:O2    | 2.15                     | 0.47              |
| 55:DA:3001:DOL:H432 | 55:DA:3001:DOL:O7  | 2.13                     | 0.47              |
| 22:DA:40:U:C4       | 22:DA:41:C:N4      | 2.83                     | 0.47              |
| 22:DA:668:A:H3'     | 22:DA:669:G:H5''   | 1.96                     | 0.47              |
| 22:DA:619:G:O6      | 26:DE:98:LYS:HE3   | 2.15                     | 0.47              |
| 28:DG:98:VAL:HG11   | 28:DG:124:GLU:HA   | 1.96                     | 0.47              |
| 32:DK:31:ARG:HB3    | 32:DK:32:TYR:CD2   | 2.49                     | 0.47              |
| 33:DL:77:ILE:CG2    | 33:DL:81:ASP:OD2   | 2.63                     | 0.47              |
| 35:DN:24:MET:HE3    | 35:DN:44:LEU:HD22  | 1.97                     | 0.47              |
| 41:DT:23:ALA:O      | 41:DT:27:SER:N     | 2.48                     | 0.47              |
| 45:DX:40:VAL:CG2    | 45:DX:45:ARG:O     | 2.63                     | 0.47              |
| 1:AA:1027:C:C5      | 1:AA:1028:C:N4     | 2.82                     | 0.47              |
| 1:AA:1305:G:HO2'    | 1:AA:1306:A:H8     | 1.60                     | 0.47              |
| 1:AA:1381:U:C5      | 1:AA:1382:C:C5     | 3.03                     | 0.47              |
| 1:AA:65:A:C2        | 1:AA:381:C:C6      | 3.03                     | 0.47              |
| 2:AB:160:ALA:O      | 2:AB:161:LEU:HB2   | 2.15                     | 0.47              |
| 2:AB:206:ALA:O      | 2:AB:210:VAL:HG22  | 2.14                     | 0.47              |
| 2:AB:94:HIS:ND1     | 2:AB:146:ASN:HB2   | 2.30                     | 0.47              |
| 7:AG:127:ALA:O      | 7:AG:130:ASN:N     | 2.46                     | 0.47              |
| 16:AP:22:ALA:HA     | 16:AP:33:ILE:CG1   | 2.43                     | 0.47              |
| 1:AA:186:C:H4'      | 20:AT:76:LYS:HB2   | 1.96                     | 0.47              |
| 48:B0:44:THR:HG23   | 48:B0:48:TYR:O     | 2.15                     | 0.47              |
| 50:B2:43:THR:O      | 50:B2:44:VAL:CB    | 2.62                     | 0.47              |
| 53:B5:122:GLY:CA    | 53:B5:146:VAL:CB   | 2.93                     | 0.47              |
| 22:BA:1384:A:H1'    | 22:BA:1405:U:C1'   | 2.45                     | 0.47              |
| 22:BA:1668:A:O2'    | 22:BA:1674:G:N7    | 2.36                     | 0.47              |
| 22:BA:1959:G:C2'    | 22:BA:1960:A:O5'   | 2.62                     | 0.47              |
| 22:BA:205:G:O2'     | 22:BA:206:U:OP2    | 2.33                     | 0.47              |
| 22:BA:309:A:C5      | 22:BA:330:A:C6     | 3.03                     | 0.47              |
| 23:BB:7:G:H5''      | 36:BO:29:HIS:CE1   | 2.50                     | 0.47              |
| 28:BG:85:LYS:CG     | 28:BG:141:ILE:HD13 | 2.45                     | 0.47              |
| 34:BM:2:LEU:O       | 34:BM:3:GLN:HB3    | 2.15                     | 0.47              |
| 46:BY:6:LEU:HD22    | 46:BY:56:LEU:HD21  | 1.97                     | 0.47              |
| 1:CA:1052:U:H5''    | 1:CA:1053:G:OP2    | 2.15                     | 0.47              |
| 1:CA:1311:A:C2      | 1:CA:1327:C:N3     | 2.83                     | 0.47              |
| 1:CA:1348:U:H4'     | 9:CI:122:ARG:CG    | 2.45                     | 0.47              |
| 1:CA:1386:G:H2'     | 1:CA:1387:G:H8     | 1.80                     | 0.47              |
| 1:CA:16:A:C6        | 1:CA:17:U:C5       | 3.02                     | 0.47              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:427:U:P       | 4:CD:13:ARG:HH22   | 2.38                     | 0.47              |
| 1:CA:581:G:N2      | 1:CA:761:G:C6      | 2.83                     | 0.47              |
| 1:CA:991:U:H4'     | 1:CA:992:U:OP1     | 2.15                     | 0.47              |
| 5:CE:38:VAL:HG11   | 5:CE:114:VAL:HA    | 1.96                     | 0.47              |
| 17:CQ:81:LYS:N     | 17:CQ:81:LYS:HD2   | 2.30                     | 0.47              |
| 17:CQ:8:LEU:HD12   | 17:CQ:8:LEU:N      | 2.29                     | 0.47              |
| 22:DA:1335:C:H2'   | 22:DA:1336:A:C8    | 2.50                     | 0.47              |
| 22:DA:1434:A:H2'   | 22:DA:1435:G:C8    | 2.50                     | 0.47              |
| 22:DA:1726:C:H2'   | 22:DA:1727:C:H6    | 1.79                     | 0.47              |
| 22:DA:1855:U:C5    | 22:DA:1856:U:C4    | 3.03                     | 0.47              |
| 22:DA:1891:G:H2'   | 22:DA:1892:C:O4'   | 2.14                     | 0.47              |
| 22:DA:200:U:C5     | 22:DA:201:C:C4     | 3.02                     | 0.47              |
| 22:DA:2043:C:H2'   | 22:DA:2043:C:O2    | 2.14                     | 0.47              |
| 22:DA:2148:G:C2    | 22:DA:2149:U:C4    | 3.03                     | 0.47              |
| 22:DA:2652:C:N4    | 22:DA:2653:U:O4    | 2.48                     | 0.47              |
| 22:DA:2732:G:O2'   | 22:DA:2733:A:H5'   | 2.15                     | 0.47              |
| 22:DA:5:A:C2       | 22:DA:2899:A:C2    | 3.03                     | 0.47              |
| 22:DA:35:G:C5      | 22:DA:454:A:C2     | 3.03                     | 0.47              |
| 25:DD:175:LEU:HD11 | 25:DD:193:VAL:HG12 | 1.97                     | 0.47              |
| 33:DL:116:VAL:HG21 | 33:DL:134:ALA:O    | 2.15                     | 0.47              |
| 33:DL:55:MET:SD    | 33:DL:59:ARG:HB3   | 2.55                     | 0.47              |
| 35:DN:106:ASP:CG   | 35:DN:106:ASP:O    | 2.51                     | 0.47              |
| 35:DN:104:ALA:O    | 35:DN:106:ASP:N    | 2.48                     | 0.47              |
| 1:AA:1009:U:H2'    | 1:AA:1010:U:C6     | 2.50                     | 0.46              |
| 1:AA:1163:A:C2     | 1:AA:1174:G:N1     | 2.82                     | 0.46              |
| 1:AA:1203:C:H4'    | 14:AN:67:THR:HG22  | 1.97                     | 0.46              |
| 1:AA:819:A:H4'     | 1:AA:820:U:OP2     | 2.15                     | 0.46              |
| 2:AB:164:ILE:O     | 2:AB:186:ILE:HG12  | 2.15                     | 0.46              |
| 2:AB:63:ARG:O      | 2:AB:64:LYS:CB     | 2.60                     | 0.46              |
| 2:AB:66:LYS:N      | 2:AB:66:LYS:HD3    | 2.30                     | 0.46              |
| 3:AC:143:ARG:CG    | 3:AC:144:LEU:HD13  | 2.44                     | 0.46              |
| 4:AD:107:PHE:CD1   | 4:AD:145:ILE:HD11  | 2.49                     | 0.46              |
| 1:AA:1377:A:C4     | 7:AG:7:ILE:HD11    | 2.49                     | 0.46              |
| 5:AE:155:ALA:HB1   | 8:AH:66:PHE:CE2    | 2.50                     | 0.46              |
| 10:AJ:54:SER:OG    | 10:AJ:55:PRO:HD2   | 2.14                     | 0.46              |
| 10:AJ:57:VAL:HG22  | 10:AJ:58:ASN:N     | 2.30                     | 0.46              |
| 12:AL:44:LYS:HB3   | 12:AL:45:PRO:HD3   | 1.96                     | 0.46              |
| 16:AP:4:ILE:HG13   | 16:AP:21:VAL:HG22  | 1.97                     | 0.46              |
| 17:AQ:46:VAL:HG13  | 17:AQ:73:TRP:C     | 2.35                     | 0.46              |
| 19:AS:40:ILE:CG1   | 19:AS:71:LEU:HD22  | 2.45                     | 0.46              |
| 50:B2:43:THR:C     | 50:B2:44:VAL:HG12  | 2.35                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 52:B4:1:MET:SD    | 52:B4:36:ARG:HB2  | 2.55                     | 0.46              |
| 53:B5:79:ALA:HB1  | 53:B5:83:LYS:HB2  | 1.97                     | 0.46              |
| 22:BA:1084:A:C5   | 22:BA:1085:A:C6   | 3.03                     | 0.46              |
| 22:BA:1855:U:C5   | 22:BA:1856:U:C5   | 3.04                     | 0.46              |
| 22:BA:190:A:C4    | 22:BA:207:A:C2    | 3.03                     | 0.46              |
| 22:BA:827:U:H2'   | 22:BA:2068:U:C2   | 2.50                     | 0.46              |
| 22:BA:2786:U:OP1  | 25:BD:70:LYS:NZ   | 2.36                     | 0.46              |
| 22:BA:2804:U:H2'  | 22:BA:2805:C:H6   | 1.80                     | 0.46              |
| 22:BA:2847:U:H2'  | 22:BA:2848:G:H5'  | 1.96                     | 0.46              |
| 22:BA:39:G:H2'    | 22:BA:40:U:C6     | 2.49                     | 0.46              |
| 22:BA:465:G:H2'   | 22:BA:466:A:C8    | 2.50                     | 0.46              |
| 23:BB:35:C:C2'    | 23:BB:36:C:H5'    | 2.44                     | 0.46              |
| 23:BB:53:A:N3     | 23:BB:53:A:H2'    | 2.31                     | 0.46              |
| 22:BA:784:G:C5'   | 24:BC:226:ASN:OD1 | 2.63                     | 0.46              |
| 25:BD:61:THR:CB   | 25:BD:63:PRO:HD2  | 2.45                     | 0.46              |
| 29:BH:91:PHE:O    | 1:CA:55:A:C2      | 2.68                     | 0.46              |
| 1:CA:157:U:O2     | 1:CA:165:G:C2     | 2.68                     | 0.46              |
| 1:CA:872:A:C4     | 1:CA:874:G:C8     | 3.02                     | 0.46              |
| 2:CB:85:LEU:O     | 2:CB:85:LEU:HD12  | 2.15                     | 0.46              |
| 11:CK:44:TRP:HA   | 11:CK:70:CYS:SG   | 2.55                     | 0.46              |
| 50:D2:44:VAL:O    | 50:D2:45:SER:OG   | 2.21                     | 0.46              |
| 50:D2:46:LYS:HD3  | 50:D2:46:LYS:C    | 2.36                     | 0.46              |
| 22:DA:1200:C:O2   | 22:DA:1246:A:C2   | 2.68                     | 0.46              |
| 22:DA:1207:C:N3   | 22:DA:1208:C:C5   | 2.83                     | 0.46              |
| 22:DA:1350:C:C2   | 22:DA:1382:G:C2   | 3.03                     | 0.46              |
| 22:DA:1682:G:N3   | 22:DA:1757:A:H1'  | 2.30                     | 0.46              |
| 22:DA:740:C:H5'   | 22:DA:1784:A:C2'  | 2.44                     | 0.46              |
| 22:DA:1833:C:N3   | 22:DA:1834:U:C4   | 2.83                     | 0.46              |
| 22:DA:2322:A:C6   | 22:DA:2323:G:C4   | 3.03                     | 0.46              |
| 22:DA:249:C:O5'   | 22:DA:2394:C:O2'  | 2.34                     | 0.46              |
| 22:DA:362:A:C8    | 22:DA:363:G:C8    | 3.04                     | 0.46              |
| 22:DA:42:A:C2     | 22:DA:438:G:C2    | 3.03                     | 0.46              |
| 22:DA:487:C:C2    | 22:DA:494:G:N2    | 2.83                     | 0.46              |
| 22:DA:708:G:H2'   | 22:DA:709:U:C6    | 2.50                     | 0.46              |
| 22:DA:727:A:C6    | 22:DA:728:G:C6    | 3.03                     | 0.46              |
| 22:DA:877:A:H2'   | 22:DA:878:A:OP2   | 2.14                     | 0.46              |
| 25:DD:150:GLN:C   | 25:DD:151:THR:O   | 2.52                     | 0.46              |
| 26:DE:1:MET:HB2   | 26:DE:16:GLU:HA   | 1.96                     | 0.46              |
| 34:DM:56:ALA:C    | 34:DM:58:LYS:H    | 2.18                     | 0.46              |
| 43:DV:38:LEU:HD23 | 43:DV:40:ILE:CD1  | 2.45                     | 0.46              |
| 1:AA:1133:G:N2    | 1:AA:1142:G:C4    | 2.83                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AA:1145:A:O2'   | 1:AA:1146:A:O5'   | 2.31                     | 0.46              |
| 1:AA:145:G:N2     | 1:AA:178:C:C2     | 2.82                     | 0.46              |
| 1:AA:2:A:C6       | 1:AA:3:A:N1       | 2.84                     | 0.46              |
| 1:AA:572:A:H5'    | 1:AA:573:A:P      | 2.56                     | 0.46              |
| 1:AA:8:A:N6       | 4:AD:202:GLU:O    | 2.46                     | 0.46              |
| 3:AC:7:PRO:HG2    | 3:AC:184:TYR:CD1  | 2.50                     | 0.46              |
| 1:AA:404:G:N7     | 4:AD:2:ALA:HB3    | 2.30                     | 0.46              |
| 4:AD:62:ARG:HG3   | 4:AD:72:PHE:CD2   | 2.50                     | 0.46              |
| 7:AG:130:ASN:HA   | 7:AG:135:VAL:HG11 | 1.96                     | 0.46              |
| 8:AH:87:LYS:HG2   | 8:AH:91:GLU:O     | 2.16                     | 0.46              |
| 10:AJ:32:THR:OG1  | 10:AJ:33:GLY:N    | 2.46                     | 0.46              |
| 10:AJ:52:LEU:HD23 | 10:AJ:62:ARG:HG2  | 1.96                     | 0.46              |
| 14:AN:46:LEU:O    | 14:AN:47:LYS:C    | 2.54                     | 0.46              |
| 10:AJ:53:ILE:HD11 | 14:AN:85:ARG:NH1  | 2.31                     | 0.46              |
| 20:AT:54:MET:HA   | 20:AT:57:ILE:HG22 | 1.96                     | 0.46              |
| 22:BA:1006:C:C2   | 22:BA:1138:G:N2   | 2.83                     | 0.46              |
| 22:BA:1635:A:C6   | 22:BA:1636:U:C2   | 3.02                     | 0.46              |
| 22:BA:1734:G:H2'  | 22:BA:1735:A:H8   | 1.80                     | 0.46              |
| 22:BA:1911:U:C4   | 22:BA:1918:A:C5   | 3.02                     | 0.46              |
| 22:BA:2558:C:O2'  | 22:BA:2559:C:H5'  | 2.15                     | 0.46              |
| 22:BA:271:G:H4'   | 22:BA:272:A:OP1   | 2.16                     | 0.46              |
| 22:BA:2790:U:H5'  | 22:BA:2893:A:N7   | 2.30                     | 0.46              |
| 22:BA:477:A:C6    | 22:BA:478:A:C6    | 3.03                     | 0.46              |
| 22:BA:697:G:H2'   | 22:BA:698:C:C6    | 2.50                     | 0.46              |
| 24:BC:209:GLY:O   | 24:BC:210:ALA:C   | 2.53                     | 0.46              |
| 27:BF:17:MET:SD   | 27:BF:25:VAL:HA   | 2.55                     | 0.46              |
| 38:BQ:62:ILE:HG23 | 38:BQ:76:TYR:CE1  | 2.50                     | 0.46              |
| 45:BX:37:ARG:NH1  | 45:BX:46:PHE:CE1  | 2.83                     | 0.46              |
| 1:CA:1202:U:H2'   | 1:CA:1203:C:O4'   | 2.15                     | 0.46              |
| 1:CA:681:A:C2     | 1:CA:710:G:N3     | 2.83                     | 0.46              |
| 1:CA:731:G:H5'    | 1:CA:766:A:H4'    | 1.97                     | 0.46              |
| 1:CA:774:G:C6     | 1:CA:775:G:C5     | 3.03                     | 0.46              |
| 5:CE:77:ASN:O     | 5:CE:80:THR:HG22  | 2.15                     | 0.46              |
| 6:CF:62:MET:O     | 6:CF:63:ASN:HB2   | 2.15                     | 0.46              |
| 7:CG:116:MET:HA   | 7:CG:119:ARG:HD3  | 1.97                     | 0.46              |
| 8:CH:66:PHE:CE2   | 8:CH:67:GLN:OE1   | 2.67                     | 0.46              |
| 1:CA:1060:U:H5'   | 10:CJ:53:ILE:HG23 | 1.98                     | 0.46              |
| 13:CM:3:ARG:HA    | 13:CM:8:ASN:O     | 2.15                     | 0.46              |
| 15:CO:3:LEU:HD13  | 15:CO:35:GLN:HG2  | 1.96                     | 0.46              |
| 13:CM:85:CYS:HB3  | 19:CS:74:PHE:CZ   | 2.50                     | 0.46              |
| 22:DA:1364:G:H2'  | 22:DA:1365:A:C5'  | 2.46                     | 0.46              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:DA:2064:C:H2'  | 22:DA:2065:C:C6    | 2.50                     | 0.46              |
| 22:DA:2079:U:C2'  | 22:DA:2080:A:O4'   | 2.62                     | 0.46              |
| 22:DA:2331:G:N2   | 22:DA:2385:C:N1    | 2.64                     | 0.46              |
| 22:DA:2566:A:N1   | 32:DK:28:SER:OG    | 2.35                     | 0.46              |
| 22:DA:276:U:O2'   | 22:DA:278:A:N7     | 2.49                     | 0.46              |
| 22:DA:2799:A:C2   | 22:DA:2801:G:H1'   | 2.50                     | 0.46              |
| 22:DA:54:G:C6     | 22:DA:55:G:N7      | 2.83                     | 0.46              |
| 22:DA:609:A:C6    | 22:DA:610:C:O2     | 2.68                     | 0.46              |
| 22:DA:618:G:C2    | 22:DA:619:G:H1'    | 2.50                     | 0.46              |
| 25:DD:56:LYS:O    | 25:DD:57:ALA:C     | 2.53                     | 0.46              |
| 27:DF:117:LEU:HB3 | 27:DF:130:MET:SD   | 2.56                     | 0.46              |
| 31:DJ:4:PHE:CD2   | 38:DQ:100:VAL:HG11 | 2.50                     | 0.46              |
| 32:DK:105:ARG:N   | 32:DK:122:VAL:OXT  | 2.48                     | 0.46              |
| 33:DL:54:GLN:HG2  | 33:DL:55:MET:N     | 2.30                     | 0.46              |
| 34:DM:136:MET:HE2 | 43:DV:57:TYR:CD2   | 2.49                     | 0.46              |
| 41:DT:7:LEU:HD21  | 41:DT:45:ALA:HB3   | 1.98                     | 0.46              |
| 42:DU:96:PHE:CE1  | 42:DU:103:ILE:HG13 | 2.51                     | 0.46              |
| 1:AA:553:A:C2'    | 1:AA:554:A:H5'     | 2.45                     | 0.46              |
| 1:AA:559:A:H2'    | 1:AA:559:A:N3      | 2.29                     | 0.46              |
| 1:AA:652:U:C4     | 1:AA:752:G:N3      | 2.83                     | 0.46              |
| 1:AA:896:C:O2'    | 1:AA:897:C:H5'     | 2.15                     | 0.46              |
| 1:AA:983:A:H5''   | 1:AA:984:C:OP2     | 2.14                     | 0.46              |
| 2:AB:132:LYS:O    | 2:AB:136:MET:HB2   | 2.15                     | 0.46              |
| 2:AB:200:ILE:O    | 2:AB:201:PRO:O     | 2.33                     | 0.46              |
| 2:AB:34:ALA:O     | 2:AB:35:ARG:C      | 2.53                     | 0.46              |
| 3:AC:113:ALA:HA   | 3:AC:200:VAL:HG21  | 1.98                     | 0.46              |
| 4:AD:122:ALA:O    | 4:AD:123:ILE:CG2   | 2.62                     | 0.46              |
| 4:AD:107:PHE:CD1  | 4:AD:145:ILE:HD13  | 2.51                     | 0.46              |
| 5:AE:116:GLU:HG2  | 5:AE:117:VAL:N     | 2.31                     | 0.46              |
| 8:AH:105:SER:O    | 8:AH:123:GLY:HA3   | 2.15                     | 0.46              |
| 8:AH:11:LEU:HD11  | 8:AH:127:CYS:CB    | 2.45                     | 0.46              |
| 14:AN:93:ILE:HD12 | 14:AN:96:LEU:HD23  | 1.96                     | 0.46              |
| 15:AO:56:LEU:HD12 | 15:AO:56:LEU:O     | 2.15                     | 0.46              |
| 17:AQ:69:LYS:O    | 17:AQ:70:THR:OG1   | 2.33                     | 0.46              |
| 20:AT:67:ILE:HG13 | 20:AT:71:LYS:CG    | 2.46                     | 0.46              |
| 21:AU:34:ARG:NE   | 21:AU:35:ARG:HB2   | 2.30                     | 0.46              |
| 53:B5:73:VAL:CG2  | 53:B5:162:ILE:CB   | 2.93                     | 0.46              |
| 53:B5:28:ARG:HG3  | 53:B5:28:ARG:O     | 2.15                     | 0.46              |
| 53:B5:78:ILE:HG22 | 53:B5:123:ALA:HA   | 1.96                     | 0.46              |
| 22:BA:1192:G:O2'  | 22:BA:1193:G:H5'   | 2.16                     | 0.46              |
| 22:BA:1886:U:O2'  | 22:BA:1887:C:H5'   | 2.15                     | 0.46              |

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| Atom-1            | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 22:BA:1958:C:C2'  | 22:BA:1959:G:H5'    | 2.45                     | 0.46              |
| 22:BA:2076:U:C4'  | 22:BA:2076:U:O2     | 2.63                     | 0.46              |
| 22:BA:2154:A:H2'  | 22:BA:2155:U:C5     | 2.51                     | 0.46              |
| 22:BA:2584:U:C2'  | 22:BA:2585:U:H5'    | 2.43                     | 0.46              |
| 22:BA:720:U:H2'   | 22:BA:721:A:C8      | 2.51                     | 0.46              |
| 22:BA:826:U:O2'   | 33:BL:53:GLY:CA     | 2.60                     | 0.46              |
| 22:BA:974:G:C8    | 22:BA:990:A:N6      | 2.81                     | 0.46              |
| 23:BB:75:G:H2'    | 23:BB:76:G:O4'      | 2.15                     | 0.46              |
| 26:BE:7:ASP:O     | 26:BE:9:GLN:N       | 2.48                     | 0.46              |
| 22:BA:2310:C:C5   | 27:BF:77:PHE:CZ     | 3.03                     | 0.46              |
| 29:BH:132:PHE:CD2 | 29:BH:142:VAL:CG2   | 2.99                     | 0.46              |
| 29:BH:80:ILE:HG21 | 29:BH:94:ILE:CG1    | 2.45                     | 0.46              |
| 22:BA:973:A:H5''  | 39:BR:81:LYS:HE3    | 1.97                     | 0.46              |
| 22:BA:927:A:O2'   | 47:BZ:39:GLU:OE2    | 2.25                     | 0.46              |
| 1:CA:999:C:H2'    | 1:CA:1000:A:C8      | 2.50                     | 0.46              |
| 1:CA:1361:G:C4    | 1:CA:1362:A:C8      | 3.03                     | 0.46              |
| 1:CA:1489:G:C5    | 1:CA:1490:U:C5      | 3.04                     | 0.46              |
| 3:CC:110:GLU:C    | 3:CC:111:LEU:HD22   | 2.35                     | 0.46              |
| 3:CC:126:ARG:O    | 3:CC:127:ARG:CB     | 2.63                     | 0.46              |
| 5:CE:109:GLY:O    | 5:CE:110:ALA:CB     | 2.63                     | 0.46              |
| 6:CF:80:PHE:O     | 6:CF:80:PHE:CG      | 2.68                     | 0.46              |
| 7:CG:14:PRO:O     | 7:CG:15:ASP:C       | 2.54                     | 0.46              |
| 19:CS:50:ALA:HB1  | 19:CS:57:HIS:HB3    | 1.98                     | 0.46              |
| 19:CS:55:ARG:NE   | 19:CS:79:THR:CG2    | 2.79                     | 0.46              |
| 49:D1:39:PHE:CG   | 49:D1:40:ASP:N      | 2.84                     | 0.46              |
| 22:DA:2370:G:O2'  | 49:D1:44:ARG:NH1    | 2.49                     | 0.46              |
| 22:DA:1362:C:H2'  | 22:DA:1363:C:C5'    | 2.46                     | 0.46              |
| 22:DA:1544:A:N6   | 22:DA:1545:A:C6     | 2.83                     | 0.46              |
| 22:DA:52:A:C2     | 22:DA:178:G:N3      | 2.83                     | 0.46              |
| 22:DA:223:A:H2'   | 22:DA:408:G:N3      | 2.31                     | 0.46              |
| 22:DA:224:U:OP2   | 22:DA:408:G:N2      | 2.48                     | 0.46              |
| 22:DA:2892:G:H5'' | 22:DA:2894:G:N2     | 2.31                     | 0.46              |
| 22:DA:2063:C:C4'  | 55:DA:3001:DOL:H343 | 2.43                     | 0.46              |
| 22:DA:593:U:C2    | 22:DA:594:U:C5      | 3.03                     | 0.46              |
| 22:DA:784:G:H5''  | 24:DC:226:ASN:OD1   | 2.14                     | 0.46              |
| 22:DA:864:G:N2    | 22:DA:913:U:C2      | 2.83                     | 0.46              |
| 24:DC:76:ALA:HB2  | 24:DC:96:TYR:CD2    | 2.49                     | 0.46              |
| 35:DN:31:HIS:O    | 35:DN:33:ILE:HG22   | 2.16                     | 0.46              |
| 37:DP:53:ARG:N    | 37:DP:57:SER:OG     | 2.48                     | 0.46              |
| 44:DW:70:GLU:O    | 44:DW:79:PHE:N      | 2.46                     | 0.46              |
| 46:DY:45:GLN:O    | 46:DY:47:ARG:N      | 2.48                     | 0.46              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:AA:1026:G:N1     | 1:AA:1035:A:C2    | 2.84                     | 0.46              |
| 1:AA:994:A:N1      | 1:AA:1047:G:H4'   | 2.30                     | 0.46              |
| 1:AA:199:A:C2      | 1:AA:200:G:C4     | 3.04                     | 0.46              |
| 1:AA:501:C:H2'     | 1:AA:502:A:C8     | 2.49                     | 0.46              |
| 1:AA:582:C:N3      | 1:AA:583:A:C8     | 2.84                     | 0.46              |
| 1:AA:73:C:HO2'     | 1:AA:74:A:C5'     | 2.28                     | 0.46              |
| 1:AA:867:G:O2'     | 1:AA:873:A:N1     | 2.38                     | 0.46              |
| 8:AH:47:GLU:N      | 8:AH:64:LYS:HG3   | 2.31                     | 0.46              |
| 10:AJ:41:PRO:O     | 10:AJ:71:LEU:O    | 2.33                     | 0.46              |
| 10:AJ:52:LEU:CB    | 14:AN:81:ARG:HE   | 2.28                     | 0.46              |
| 11:AK:112:ASP:HB2  | 21:AU:20:LYS:HD2  | 1.97                     | 0.46              |
| 11:AK:23:ILE:HD11  | 11:AK:86:VAL:HG13 | 1.97                     | 0.46              |
| 20:AT:68:HIS:C     | 20:AT:69:LYS:HG3  | 2.34                     | 0.46              |
| 33:BL:57:LEU:HD22  | 51:B3:54:ASP:HB3  | 1.98                     | 0.46              |
| 22:BA:1087:G:C2'   | 22:BA:1089:A:H1'  | 2.45                     | 0.46              |
| 22:BA:118:A:C8     | 22:BA:119:A:C8    | 3.03                     | 0.46              |
| 22:BA:1293:C:H2'   | 22:BA:1294:U:O4'  | 2.15                     | 0.46              |
| 22:BA:1533:C:H5'   | 22:BA:1534:U:OP2  | 2.15                     | 0.46              |
| 22:BA:1606:C:O2'   | 22:BA:1607:C:O5'  | 2.31                     | 0.46              |
| 22:BA:1871:A:C8    | 22:BA:1872:A:C6   | 3.03                     | 0.46              |
| 22:BA:2233:U:H2'   | 22:BA:2234:G:C8   | 2.50                     | 0.46              |
| 22:BA:2410:G:C2    | 22:BA:2411:A:H1'  | 2.50                     | 0.46              |
| 22:BA:25:U:H2'     | 22:BA:26:G:H5'    | 1.97                     | 0.46              |
| 22:BA:307:G:N2     | 22:BA:309:A:H3'   | 2.30                     | 0.46              |
| 22:BA:27:G:N2      | 22:BA:512:G:H1'   | 2.29                     | 0.46              |
| 22:BA:713:G:C6     | 22:BA:714:U:C4    | 3.03                     | 0.46              |
| 22:BA:776:G:H4'    | 22:BA:777:G:O5'   | 2.15                     | 0.46              |
| 24:BC:195:VAL:HG12 | 24:BC:196:GLY:N   | 2.29                     | 0.46              |
| 25:BD:61:THR:HB    | 25:BD:63:PRO:HD2  | 1.97                     | 0.46              |
| 26:BE:108:ILE:HG13 | 26:BE:109:LEU:N   | 2.29                     | 0.46              |
| 27:BF:4:LEU:HD22   | 27:BF:173:PHE:CD2 | 2.51                     | 0.46              |
| 27:BF:58:ALA:O     | 27:BF:61:SER:O    | 2.34                     | 0.46              |
| 42:BU:73:PHE:CZ    | 42:BU:78:GLY:HA2  | 2.50                     | 0.46              |
| 42:BU:4:LYS:O      | 42:BU:83:VAL:HG21 | 2.16                     | 0.46              |
| 1:CA:1279:G:H5''   | 10:CJ:9:ARG:NH2   | 2.30                     | 0.46              |
| 1:CA:1521:C:C2     | 1:CA:1522:U:C5    | 3.03                     | 0.46              |
| 1:CA:155:A:C2      | 1:CA:167:A:C5     | 3.03                     | 0.46              |
| 1:CA:955:U:H2'     | 1:CA:956:U:O4'    | 2.14                     | 0.46              |
| 1:CA:957:U:O3'     | 19:CS:79:THR:OG1  | 2.33                     | 0.46              |
| 2:CB:167:ASP:HA    | 2:CB:170:HIS:HB3  | 1.97                     | 0.46              |
| 4:CD:142:VAL:HG12  | 4:CD:181:THR:OG1  | 2.16                     | 0.46              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 13:CM:40:ALA:O    | 13:CM:41:GLU:C     | 2.54                     | 0.46              |
| 13:CM:91:HIS:O    | 13:CM:109:ARG:NH2  | 2.49                     | 0.46              |
| 15:CO:39:LEU:O    | 15:CO:42:HIS:HB3   | 2.16                     | 0.46              |
| 20:CT:21:ASN:O    | 20:CT:25:ARG:HB3   | 2.15                     | 0.46              |
| 22:DA:1208:C:C5   | 22:DA:1209:U:C5    | 3.03                     | 0.46              |
| 22:DA:1248:G:C4   | 38:DQ:3:ARG:HG3    | 2.50                     | 0.46              |
| 22:DA:1347:A:C5   | 22:DA:1348:C:C5    | 3.03                     | 0.46              |
| 22:DA:1351:C:C2   | 22:DA:1381:G:C2    | 3.04                     | 0.46              |
| 22:DA:1678:A:C4   | 22:DA:1679:A:C8    | 3.03                     | 0.46              |
| 22:DA:1753:G:N1   | 22:DA:1756:G:C2    | 2.84                     | 0.46              |
| 22:DA:2056:G:N3   | 22:DA:2056:G:H2'   | 2.30                     | 0.46              |
| 22:DA:2209:G:C2   | 22:DA:2216:G:C2    | 3.04                     | 0.46              |
| 22:DA:2741:A:H2'  | 22:DA:2742:G:H5'   | 1.98                     | 0.46              |
| 22:DA:2748:A:C2   | 22:DA:2757:A:C5    | 3.03                     | 0.46              |
| 22:DA:311:A:OP1   | 22:DA:332:A:C2     | 2.69                     | 0.46              |
| 22:DA:349:U:C2'   | 22:DA:350:G:H5'    | 2.45                     | 0.46              |
| 22:DA:398:C:OP2   | 45:DX:53:ALA:HB3   | 2.16                     | 0.46              |
| 22:DA:528:A:N1    | 22:DA:2042:A:H2'   | 2.30                     | 0.46              |
| 22:DA:630:G:H3'   | 22:DA:631:A:H5''   | 1.97                     | 0.46              |
| 22:DA:883:G:N2    | 22:DA:894:U:O2     | 2.49                     | 0.46              |
| 24:DC:72:ASP:OD1  | 24:DC:189:ARG:NH1  | 2.48                     | 0.46              |
| 24:DC:246:THR:C   | 24:DC:248:TRP:N    | 2.69                     | 0.46              |
| 29:DH:41:LYS:O    | 29:DH:44:ILE:HG12  | 2.15                     | 0.46              |
| 30:DI:49:ILE:O    | 30:DI:50:GLU:HB2   | 2.16                     | 0.46              |
| 33:DL:95:LEU:O    | 33:DL:100:ILE:HG23 | 2.16                     | 0.46              |
| 35:DN:29:VAL:HG13 | 35:DN:83:LEU:HD11  | 1.96                     | 0.46              |
| 37:DP:65:SER:O    | 37:DP:66:ASN:C     | 2.53                     | 0.46              |
| 46:DY:18:LEU:O    | 46:DY:22:LEU:HB3   | 2.15                     | 0.46              |
| 1:AA:1253:G:C4    | 1:AA:1254:A:C8     | 3.03                     | 0.46              |
| 1:AA:36:C:H2'     | 1:AA:37:U:O4'      | 2.15                     | 0.46              |
| 1:AA:67:C:O2'     | 1:AA:171:A:H1'     | 2.15                     | 0.46              |
| 1:AA:832:G:C4     | 1:AA:833:G:C8      | 3.03                     | 0.46              |
| 1:AA:859:G:H2'    | 1:AA:860:A:H8      | 1.76                     | 0.46              |
| 1:AA:919:A:O2'    | 1:AA:920:U:H5'     | 2.15                     | 0.46              |
| 2:AB:163:VAL:HG22 | 2:AB:185:ALA:HB1   | 1.98                     | 0.46              |
| 2:AB:50:PHE:CD2   | 2:AB:51:ASN:OD1    | 2.69                     | 0.46              |
| 3:AC:84:VAL:HG13  | 3:AC:101:ILE:HG21  | 1.98                     | 0.46              |
| 3:AC:130:PHE:CZ   | 3:AC:131:ARG:HD3   | 2.51                     | 0.46              |
| 4:AD:124:MET:HG3  | 4:AD:146:ARG:HG2   | 1.97                     | 0.46              |
| 5:AE:136:VAL:HG22 | 5:AE:137:VAL:N     | 2.30                     | 0.46              |
| 6:AF:45:ARG:HG2   | 6:AF:46:GLN:N      | 2.30                     | 0.46              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 7:AG:71:PRO:O      | 7:AG:96:ARG:HG3   | 2.16                     | 0.46              |
| 11:AK:35:THR:OG1   | 11:AK:41:ALA:N    | 2.48                     | 0.46              |
| 12:AL:29:GLN:HB2   | 12:AL:82:ILE:O    | 2.15                     | 0.46              |
| 17:AQ:17:MET:CG    | 17:AQ:20:SER:HB3  | 2.46                     | 0.46              |
| 48:B0:13:ARG:O     | 48:B0:17:ARG:HG3  | 2.15                     | 0.46              |
| 22:BA:1190:G:OP1   | 33:BL:32:GLY:CA   | 2.62                     | 0.46              |
| 22:BA:198:C:O5'    | 22:BA:198:C:H6    | 1.98                     | 0.46              |
| 22:BA:197:A:H62    | 22:BA:2430:A:H2'  | 1.81                     | 0.46              |
| 22:BA:2551:C:OP1   | 57:BA:3434:HOH:O  | 2.21                     | 0.46              |
| 22:BA:422:A:C2     | 22:BA:423:A:C4    | 3.04                     | 0.46              |
| 22:BA:548:G:O2'    | 22:BA:549:G:C2    | 2.67                     | 0.46              |
| 22:BA:616:A:H2'    | 22:BA:617:G:O4'   | 2.16                     | 0.46              |
| 22:BA:780:G:H2'    | 22:BA:782:A:N7    | 2.31                     | 0.46              |
| 23:BB:116:G:H4'    | 36:BO:54:VAL:CG1  | 2.44                     | 0.46              |
| 22:BA:1820:U:O2    | 24:BC:200:HIS:HB3 | 2.15                     | 0.46              |
| 25:BD:103:ASP:OD2  | 25:BD:104:VAL:N   | 2.49                     | 0.46              |
| 27:BF:104:ILE:HG22 | 27:BF:176:PRO:CD  | 2.46                     | 0.46              |
| 29:BH:37:VAL:CG2   | 29:BH:38:PRO:HD2  | 2.45                     | 0.46              |
| 1:CA:1157:A:H5'    | 1:CA:1158:C:C6    | 2.50                     | 0.46              |
| 1:CA:295:C:C4      | 1:CA:296:U:C5     | 3.03                     | 0.46              |
| 1:CA:373:A:O2'     | 1:CA:374:A:H5'    | 2.16                     | 0.46              |
| 1:CA:414:A:C2      | 1:CA:415:A:C4     | 3.03                     | 0.46              |
| 1:CA:421:U:C4'     | 1:CA:421:U:OP1    | 2.63                     | 0.46              |
| 1:CA:674:G:OP1     | 6:CF:86:ARG:NH2   | 2.44                     | 0.46              |
| 1:CA:756:C:H2'     | 1:CA:757:U:O5'    | 2.16                     | 0.46              |
| 3:CC:36:ASP:C      | 3:CC:38:LYS:H     | 2.19                     | 0.46              |
| 9:CI:56:ASP:C      | 9:CI:57:MET:HG3   | 2.36                     | 0.46              |
| 49:D1:4:GLY:O      | 49:D1:6:ARG:N     | 2.48                     | 0.46              |
| 22:DA:1268:A:H2'   | 22:DA:1269:A:O4'  | 2.16                     | 0.46              |
| 22:DA:1289:C:O2'   | 22:DA:1330:C:H4'  | 2.15                     | 0.46              |
| 22:DA:1438:U:C4    | 22:DA:1552:A:C2   | 3.04                     | 0.46              |
| 22:DA:1833:C:C4    | 22:DA:1834:U:C4   | 3.04                     | 0.46              |
| 22:DA:2201:G:H2'   | 22:DA:2202:U:C6   | 2.51                     | 0.46              |
| 22:DA:2199:A:C5    | 22:DA:2225:A:N1   | 2.84                     | 0.46              |
| 22:DA:476:G:O4'    | 22:DA:505:A:C2    | 2.69                     | 0.46              |
| 22:DA:585:G:H2'    | 22:DA:586:A:N7    | 2.31                     | 0.46              |
| 22:DA:777:G:N3     | 22:DA:778:G:C8    | 2.83                     | 0.46              |
| 23:DB:100:G:H2'    | 23:DB:101:A:O4'   | 2.15                     | 0.46              |
| 24:DC:68:LYS:HG2   | 24:DC:151:GLY:HA2 | 1.97                     | 0.46              |
| 22:DA:1799:G:O2'   | 24:DC:180:GLU:OE2 | 2.26                     | 0.46              |
| 24:DC:260:ASN:OD1  | 24:DC:263:THR:N   | 2.45                     | 0.46              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:DD:18:ASP:OD2  | 25:DD:18:ASP:N     | 2.49                     | 0.46              |
| 27:DF:163:ASP:N   | 27:DF:163:ASP:OD1  | 2.49                     | 0.46              |
| 32:DK:121:GLU:HG2 | 32:DK:122:VAL:HG23 | 1.97                     | 0.46              |
| 33:DL:59:ARG:CZ   | 33:DL:59:ARG:HB3   | 2.44                     | 0.46              |
| 36:DO:27:VAL:HG21 | 36:DO:40:ILE:HD12  | 1.98                     | 0.46              |
| 36:DO:51:ALA:HB1  | 36:DO:77:ALA:CB    | 2.45                     | 0.46              |
| 42:DU:9:ASP:OD2   | 42:DU:10:GLU:O     | 2.34                     | 0.46              |
| 46:DY:1:MET:HA    | 46:DY:4:LYS:HB2    | 1.97                     | 0.46              |
| 46:DY:21:LEU:HA   | 46:DY:25:GLN:HB3   | 1.98                     | 0.46              |
| 1:AA:1084:G:C5    | 1:AA:1085:U:C4     | 3.02                     | 0.46              |
| 1:AA:1107:C:C2    | 1:AA:1108:G:C8     | 3.04                     | 0.46              |
| 1:AA:515:G:O6     | 57:AA:1847:HOH:O   | 2.21                     | 0.46              |
| 1:AA:529:G:H4'    | 1:AA:533:A:C2      | 2.50                     | 0.46              |
| 5:AE:14:LYS:NZ    | 5:AE:116:GLU:OE2   | 2.48                     | 0.46              |
| 9:AI:127:PHE:O    | 9:AI:127:PHE:CD2   | 2.69                     | 0.46              |
| 9:AI:20:PHE:O     | 9:AI:63:LEU:HA     | 2.15                     | 0.46              |
| 16:AP:20:VAL:HG21 | 16:AP:32:PHE:CG    | 2.51                     | 0.46              |
| 53:B5:36:ALA:O    | 53:B5:37:LYS:HB2   | 2.15                     | 0.46              |
| 22:BA:1062:G:OP1  | 22:BA:1070:A:H4'   | 2.16                     | 0.46              |
| 22:BA:140:C:O2    | 22:BA:140:C:O4'    | 2.34                     | 0.46              |
| 22:BA:1916:A:O3'  | 22:BA:1917:U:H4'   | 2.16                     | 0.46              |
| 22:BA:1925:C:C4'  | 22:BA:1926:U:OP1   | 2.55                     | 0.46              |
| 22:BA:528:A:H2    | 22:BA:2043:C:C5'   | 2.28                     | 0.46              |
| 22:BA:2080:A:H5'  | 45:BX:19:SER:HB2   | 1.97                     | 0.46              |
| 22:BA:2190:G:N1   | 22:BA:2191:A:C4    | 2.84                     | 0.46              |
| 22:BA:2284:A:C5   | 22:BA:2285:C:C5    | 3.03                     | 0.46              |
| 22:BA:2518:A:H2'  | 22:BA:2518:A:N3    | 2.30                     | 0.46              |
| 22:BA:2637:U:H2'  | 22:BA:2638:G:H5'   | 1.97                     | 0.46              |
| 24:BC:88:SER:HB2  | 24:BC:200:HIS:CD2  | 2.51                     | 0.46              |
| 26:BE:134:LEU:O   | 26:BE:135:ALA:C    | 2.53                     | 0.46              |
| 30:BI:57:VAL:HG22 | 30:BI:58:VAL:N     | 2.30                     | 0.46              |
| 31:BJ:31:GLU:HG3  | 31:BJ:142:ILE:HD11 | 1.97                     | 0.46              |
| 1:AA:345:C:O2'    | 32:BK:116:ILE:CD1  | 2.63                     | 0.46              |
| 37:BP:58:ALA:HB1  | 37:BP:74:PHE:O     | 2.15                     | 0.46              |
| 22:BA:445:C:OP1   | 38:BQ:2:ALA:N      | 2.48                     | 0.46              |
| 40:BS:36:LEU:CD1  | 40:BS:47:VAL:HG12  | 2.46                     | 0.46              |
| 1:CA:146:G:N2     | 1:CA:147:G:H1'     | 2.30                     | 0.46              |
| 1:CA:577:G:C8     | 1:CA:816:A:C2      | 3.03                     | 0.46              |
| 7:CG:123:GLU:OE1  | 7:CG:123:GLU:HA    | 2.16                     | 0.46              |
| 9:CI:90:TYR:O     | 9:CI:91:ASP:O      | 2.34                     | 0.46              |
| 11:CK:100:LEU:O   | 11:CK:103:ALA:N    | 2.48                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:CN:61:ARG:O    | 14:CN:62:ASN:CB   | 2.64                     | 0.46              |
| 10:CJ:53:ILE:HD11 | 14:CN:85:ARG:NH1  | 2.31                     | 0.46              |
| 49:D1:19:HIS:C    | 49:D1:19:HIS:CD2  | 2.89                     | 0.46              |
| 22:DA:2477:U:O4   | 52:D4:10:LEU:HD21 | 2.16                     | 0.46              |
| 22:DA:1231:U:H2'  | 22:DA:1232:G:C8   | 2.51                     | 0.46              |
| 22:DA:1281:G:C2'  | 22:DA:1282:U:H5'  | 2.45                     | 0.46              |
| 22:DA:1306:C:C2   | 22:DA:1307:A:C8   | 3.03                     | 0.46              |
| 22:DA:1593:A:O2'  | 22:DA:1594:U:H5'  | 2.15                     | 0.46              |
| 22:DA:744:U:H4'   | 22:DA:1658:C:H4'  | 1.98                     | 0.46              |
| 22:DA:1709:U:H2'  | 22:DA:1710:G:C8   | 2.51                     | 0.46              |
| 22:DA:1926:U:H1'  | 22:DA:1929:G:C6   | 2.51                     | 0.46              |
| 22:DA:2170:A:C2   | 22:DA:2171:A:C6   | 3.03                     | 0.46              |
| 22:DA:2503:A:H5'  | 22:DA:2503:A:N3   | 2.31                     | 0.46              |
| 22:DA:2511:U:C4   | 22:DA:2512:C:C5   | 3.04                     | 0.46              |
| 22:DA:1662:U:O2   | 22:DA:2687:U:C5'  | 2.64                     | 0.46              |
| 22:DA:2848:G:OP2  | 37:DP:95:ALA:N    | 2.48                     | 0.46              |
| 22:DA:2852:G:H2'  | 22:DA:2853:C:O4'  | 2.15                     | 0.46              |
| 22:DA:40:U:C5     | 22:DA:41:C:N4     | 2.83                     | 0.46              |
| 22:DA:927:A:H2'   | 22:DA:928:A:C8    | 2.51                     | 0.46              |
| 24:DC:107:PRO:HB3 | 24:DC:142:HIS:CE1 | 2.49                     | 0.46              |
| 24:DC:87:ARG:CZ   | 24:DC:87:ARG:HB3  | 2.44                     | 0.46              |
| 27:DF:4:LEU:O     | 27:DF:8:TYR:HB3   | 2.15                     | 0.46              |
| 35:DN:85:PRO:O    | 35:DN:86:ARG:C    | 2.52                     | 0.46              |
| 40:DS:29:VAL:HG11 | 40:DS:55:ILE:HD11 | 1.97                     | 0.46              |
| 1:AA:1070:U:O2    | 1:AA:1071:C:C6    | 2.68                     | 0.46              |
| 1:AA:1075:U:OP1   | 2:AB:102:THR:HG21 | 2.15                     | 0.46              |
| 1:AA:1311:A:H2'   | 1:AA:1312:G:O5'   | 2.16                     | 0.46              |
| 1:AA:670:G:C2'    | 1:AA:671:G:O5'    | 2.63                     | 0.46              |
| 1:AA:849:G:C6     | 1:AA:850:U:N3     | 2.84                     | 0.46              |
| 2:AB:222:ARG:NH1  | 2:AB:222:ARG:HB3  | 2.31                     | 0.46              |
| 3:AC:149:ILE:HG12 | 3:AC:150:LYS:N    | 2.30                     | 0.46              |
| 5:AE:82:GLN:OE1   | 5:AE:148:ASN:O    | 2.33                     | 0.46              |
| 12:AL:3:THR:HG22  | 12:AL:4:VAL:N     | 2.30                     | 0.46              |
| 21:AU:29:LEU:HD23 | 21:AU:29:LEU:O    | 2.16                     | 0.46              |
| 21:AU:53:VAL:O    | 21:AU:54:LYS:HB2  | 2.15                     | 0.46              |
| 52:B4:10:LEU:HD12 | 52:B4:33:HIS:CD2  | 2.51                     | 0.46              |
| 53:B5:200:HIS:O   | 53:B5:201:LYS:C   | 2.54                     | 0.46              |
| 22:BA:1107:G:H2'  | 22:BA:1108:U:O4'  | 2.15                     | 0.46              |
| 22:BA:1157:G:N2   | 22:BA:1158:C:C2   | 2.84                     | 0.46              |
| 22:BA:1188:U:C2'  | 22:BA:1189:A:H5'  | 2.46                     | 0.46              |
| 22:BA:170:U:H2'   | 22:BA:171:U:H6    | 1.79                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:BA:1956:U:H2'   | 22:BA:1957:C:H5'   | 1.98                     | 0.46              |
| 22:BA:323:C:C4     | 22:BA:333:G:C8     | 3.04                     | 0.46              |
| 22:BA:481:G:C2     | 22:BA:507:A:N3     | 2.83                     | 0.46              |
| 22:BA:637:A:H4'    | 22:BA:638:G:O5'    | 2.15                     | 0.46              |
| 22:BA:783:A:H2'    | 22:BA:784:G:O5'    | 2.15                     | 0.46              |
| 23:BB:34:A:N3      | 23:BB:36:C:N4      | 2.61                     | 0.46              |
| 24:BC:142:HIS:C    | 24:BC:142:HIS:CD2  | 2.89                     | 0.46              |
| 24:BC:161:TYR:CD2  | 24:BC:194:GLU:HG2  | 2.51                     | 0.46              |
| 25:BD:186:LEU:HD21 | 37:BP:4:ILE:HG21   | 1.97                     | 0.46              |
| 29:BH:94:ILE:HG23  | 29:BH:98:ASP:HB2   | 1.98                     | 0.46              |
| 32:BK:66:LYS:O     | 32:BK:66:LYS:HE3   | 2.16                     | 0.46              |
| 35:BN:32:GLU:OE1   | 35:BN:118:ARG:HA   | 2.14                     | 0.46              |
| 37:BP:29:LYS:HD3   | 37:BP:40:LEU:HD23  | 1.98                     | 0.46              |
| 1:CA:1009:U:C2     | 1:CA:1021:A:N6     | 2.84                     | 0.46              |
| 1:CA:1105:A:C2     | 1:CA:1106:G:C5     | 3.04                     | 0.46              |
| 1:CA:1259:C:N4     | 1:CA:1260:G:C4     | 2.84                     | 0.46              |
| 1:CA:505:G:C2      | 1:CA:506:G:C5      | 3.04                     | 0.46              |
| 1:CA:862:C:N3      | 1:CA:863:U:C5      | 2.83                     | 0.46              |
| 2:CB:166:ALA:HB2   | 2:CB:187:VAL:HB    | 1.98                     | 0.46              |
| 5:CE:137:VAL:O     | 5:CE:138:ARG:CG    | 2.64                     | 0.46              |
| 6:CF:93:LYS:HD3    | 6:CF:93:LYS:N      | 2.31                     | 0.46              |
| 9:CI:57:MET:HA     | 9:CI:60:LYS:HB3    | 1.98                     | 0.46              |
| 1:CA:718:A:C4      | 11:CK:118:HIS:CD2  | 3.03                     | 0.46              |
| 16:CP:23:ASP:OD2   | 16:CP:25:ARG:HG3   | 2.16                     | 0.46              |
| 16:CP:6:LEU:CD1    | 16:CP:71:VAL:CG2   | 2.93                     | 0.46              |
| 14:CN:46:LEU:HG    | 19:CS:10:PHE:CD2   | 2.51                     | 0.46              |
| 51:D3:31:HIS:CE1   | 51:D3:32:ILE:HD12  | 2.50                     | 0.46              |
| 22:DA:1361:G:C6    | 22:DA:1362:C:C5    | 3.04                     | 0.46              |
| 22:DA:1332:G:C6    | 22:DA:1609:A:N7    | 2.84                     | 0.46              |
| 22:DA:1677:A:N6    | 22:DA:1678:A:C6    | 2.83                     | 0.46              |
| 22:DA:1845:G:OP1   | 24:DC:256:LYS:NZ   | 2.43                     | 0.46              |
| 22:DA:2010:G:C6    | 22:DA:2011:U:N3    | 2.84                     | 0.46              |
| 22:DA:2209:G:C6    | 22:DA:2210:U:C4    | 3.03                     | 0.46              |
| 22:DA:2318:G:C6    | 22:DA:2319:G:C6    | 3.04                     | 0.46              |
| 22:DA:27:G:HO2'    | 22:DA:28:A:P       | 2.34                     | 0.46              |
| 22:DA:337:C:C2     | 22:DA:338:G:H1'    | 2.51                     | 0.46              |
| 22:DA:412:A:H2'    | 22:DA:413:C:H5'    | 1.97                     | 0.46              |
| 22:DA:600:G:C5     | 22:DA:601:C:C4     | 3.04                     | 0.46              |
| 22:DA:58:G:C4      | 22:DA:70:G:N2      | 2.83                     | 0.46              |
| 23:DB:52:A:C5      | 36:DO:33:ARG:NH2   | 2.83                     | 0.46              |
| 28:DG:167:GLU:CG   | 28:DG:169:VAL:HG23 | 2.45                     | 0.46              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 29:DH:34:GLY:O    | 29:DH:35:LYS:CG    | 2.64                     | 0.46              |
| 29:DH:60:GLU:HA   | 29:DH:60:GLU:OE2   | 2.15                     | 0.46              |
| 30:DI:37:GLU:OE1  | 30:DI:65:ARG:NH2   | 2.49                     | 0.46              |
| 42:DU:12:ILE:CG2  | 42:DU:80:ALA:HB2   | 2.46                     | 0.46              |
| 42:DU:33:LYS:HB3  | 42:DU:64:ALA:HB1   | 1.97                     | 0.46              |
| 47:DZ:7:ILE:O     | 47:DZ:36:VAL:N     | 2.49                     | 0.46              |
| 1:AA:102:G:N1     | 1:AA:103:U:C4      | 2.84                     | 0.46              |
| 1:AA:1053:G:H4'   | 1:AA:1054:C:H5''   | 1.98                     | 0.46              |
| 1:AA:188:C:O2     | 1:AA:188:C:C2'     | 2.63                     | 0.46              |
| 1:AA:207:C:H2'    | 1:AA:208:U:O2      | 2.16                     | 0.46              |
| 1:AA:546:A:P      | 4:AD:69:GLU:HB2    | 2.56                     | 0.46              |
| 1:AA:1190:G:OP2   | 3:AC:5:VAL:HB      | 2.16                     | 0.46              |
| 3:AC:64:ILE:CG2   | 3:AC:99:ALA:HB2    | 2.46                     | 0.46              |
| 4:AD:26:ARG:HD2   | 4:AD:31:LYS:CE     | 2.46                     | 0.46              |
| 5:AE:45:ARG:HA    | 5:AE:72:ILE:O      | 2.16                     | 0.46              |
| 5:AE:148:ASN:ND2  | 8:AH:73:GLU:OE2    | 2.49                     | 0.46              |
| 9:AI:120:LYS:HG3  | 9:AI:123:ARG:HB2   | 1.97                     | 0.46              |
| 10:AJ:73:LEU:O    | 10:AJ:74:VAL:CB    | 2.64                     | 0.46              |
| 11:AK:102:ALA:O   | 11:AK:103:ALA:C    | 2.54                     | 0.46              |
| 13:AM:11:ASP:CG   | 13:AM:45:ILE:HG12  | 2.37                     | 0.46              |
| 13:AM:45:ILE:O    | 13:AM:45:ILE:CG2   | 2.63                     | 0.46              |
| 16:AP:23:ASP:C    | 16:AP:23:ASP:OD1   | 2.54                     | 0.46              |
| 1:AA:275:G:O3'    | 17:AQ:17:MET:HE2   | 2.15                     | 0.46              |
| 17:AQ:48:ASP:OD2  | 17:AQ:48:ASP:O     | 2.34                     | 0.46              |
| 17:AQ:80:GLU:C    | 17:AQ:81:LYS:HD3   | 2.36                     | 0.46              |
| 19:AS:3:ARG:O     | 19:AS:4:SER:HB2    | 2.15                     | 0.46              |
| 21:AU:12:PHE:CD1  | 21:AU:16:LEU:HD11  | 2.50                     | 0.46              |
| 21:AU:47:ARG:HE   | 21:AU:47:ARG:HA    | 1.81                     | 0.46              |
| 22:BA:1174:U:O2   | 22:BA:1174:U:O4'   | 2.33                     | 0.46              |
| 22:BA:1266:G:OP2  | 48:B0:17:ARG:NE    | 2.45                     | 0.46              |
| 22:BA:1381:G:H1'  | 22:BA:1571:A:N1    | 2.31                     | 0.46              |
| 22:BA:189:G:P     | 45:BX:26:LYS:HD2   | 2.55                     | 0.46              |
| 22:BA:2256:G:O2'  | 22:BA:2257:U:H5'   | 2.15                     | 0.46              |
| 22:BA:251:A:H2'   | 22:BA:252:G:O4'    | 2.16                     | 0.46              |
| 22:BA:25:U:C2'    | 22:BA:26:G:H5'     | 2.46                     | 0.46              |
| 22:BA:310:A:O2'   | 22:BA:311:A:P      | 2.73                     | 0.46              |
| 22:BA:340:A:H2'   | 22:BA:341:C:O4'    | 2.15                     | 0.46              |
| 22:BA:947:A:O2'   | 22:BA:984:A:H2     | 1.97                     | 0.46              |
| 27:BF:2:ALA:HB2   | 27:BF:94:GLU:OE1   | 2.15                     | 0.46              |
| 29:BH:90:LEU:HD23 | 29:BH:93:SER:HA    | 1.97                     | 0.46              |
| 30:BI:79:LEU:HD22 | 30:BI:109:ILE:HG23 | 1.97                     | 0.46              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 33:BL:101:ILE:HG13 | 33:BL:102:GLY:N   | 2.30                     | 0.46              |
| 39:BR:39:LEU:CA    | 39:BR:49:ILE:HG23 | 2.45                     | 0.46              |
| 1:CA:110:C:H2'     | 1:CA:111:G:O4'    | 2.16                     | 0.46              |
| 1:CA:1157:A:C5     | 1:CA:1180:A:C6    | 3.03                     | 0.46              |
| 1:CA:1386:G:C2     | 1:CA:1387:G:N7    | 2.84                     | 0.46              |
| 1:CA:170:U:O2'     | 1:CA:171:A:H5'    | 2.15                     | 0.46              |
| 1:CA:461:A:H2'     | 1:CA:462:G:O4'    | 2.16                     | 0.46              |
| 1:CA:513:C:H2'     | 1:CA:514:C:C6     | 2.51                     | 0.46              |
| 1:CA:731:G:O2'     | 1:CA:732:C:H5'    | 2.16                     | 0.46              |
| 1:CA:802:A:C2      | 1:CA:803:G:C1'    | 2.98                     | 0.46              |
| 1:CA:811:C:C4      | 1:CA:812:G:C6     | 3.04                     | 0.46              |
| 2:CB:175:GLU:O     | 2:CB:179:LEU:HD22 | 2.15                     | 0.46              |
| 4:CD:36:GLN:O      | 4:CD:37:ALA:HB2   | 2.15                     | 0.46              |
| 14:CN:46:LEU:CD2   | 19:CS:10:PHE:CD2  | 2.99                     | 0.46              |
| 22:DA:1545:A:H2'   | 22:DA:1546:G:O4'  | 2.15                     | 0.46              |
| 22:DA:160:A:C6     | 22:DA:161:A:C6    | 3.04                     | 0.46              |
| 22:DA:1712:U:O4    | 22:DA:1713:A:C2   | 2.69                     | 0.46              |
| 22:DA:1870:C:C3'   | 22:DA:1871:A:H5'  | 2.46                     | 0.46              |
| 22:DA:1936:A:H2    | 22:DA:1943:U:H3   | 1.63                     | 0.46              |
| 22:DA:2345:G:N3    | 22:DA:2381:A:H2'  | 2.30                     | 0.46              |
| 22:DA:2412:A:H3'   | 22:DA:2413:G:H8   | 1.80                     | 0.46              |
| 22:DA:2715:C:C4    | 22:DA:2716:C:C5   | 3.04                     | 0.46              |
| 22:DA:2804:U:C4    | 22:DA:2805:C:C4   | 3.03                     | 0.46              |
| 22:DA:349:U:O2'    | 22:DA:350:G:H5'   | 2.15                     | 0.46              |
| 22:DA:36:G:H4'     | 22:DA:451:U:C2    | 2.51                     | 0.46              |
| 22:DA:500:G:N2     | 22:DA:502:A:C8    | 2.83                     | 0.46              |
| 22:DA:579:G:C2     | 22:DA:1262:A:C5   | 3.04                     | 0.46              |
| 22:DA:695:G:C6     | 22:DA:768:G:C5    | 3.04                     | 0.46              |
| 35:DN:71:ARG:HG3   | 35:DN:71:ARG:HH21 | 1.81                     | 0.46              |
| 37:DP:75:GLN:HB2   | 37:DP:78:SER:HB2  | 1.98                     | 0.46              |
| 38:DQ:90:ILE:CG2   | 38:DQ:94:ILE:CG2  | 2.94                     | 0.46              |
| 40:DS:66:ILE:O     | 40:DS:69:LEU:HB2  | 2.16                     | 0.46              |
| 1:AA:1048:G:N3     | 1:AA:1050:G:C8    | 2.83                     | 0.46              |
| 1:AA:202:G:C2      | 1:AA:216:U:O2     | 2.69                     | 0.46              |
| 1:AA:258:G:C5      | 1:AA:259:G:C8     | 3.03                     | 0.46              |
| 1:AA:273:U:H2'     | 1:AA:274:A:H5'    | 1.97                     | 0.46              |
| 1:AA:464:U:N3      | 1:AA:466:A:H5''   | 2.31                     | 0.46              |
| 1:AA:587:G:N2      | 1:AA:755:G:C8     | 2.84                     | 0.46              |
| 1:AA:731:G:OP1     | 1:AA:766:A:H1'    | 2.15                     | 0.46              |
| 1:AA:773:G:H2'     | 1:AA:774:G:O4'    | 2.15                     | 0.46              |
| 1:AA:787:A:C5      | 1:AA:788:U:C5     | 3.04                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:AD:34:ILE:HG12   | 4:AD:35:GLU:N      | 2.30                     | 0.46              |
| 1:AA:1080:A:OP1    | 5:AE:52:LYS:HE3    | 2.16                     | 0.46              |
| 7:AG:13:LEU:HA     | 7:AG:14:PRO:HD2    | 1.86                     | 0.46              |
| 7:AG:48:GLU:O      | 7:AG:51:ALA:HB3    | 2.15                     | 0.46              |
| 8:AH:10:MET:HE1    | 8:AH:33:LYS:CB     | 2.45                     | 0.46              |
| 10:AJ:91:ASP:O     | 10:AJ:92:LEU:HD12  | 2.15                     | 0.46              |
| 11:AK:55:SER:O     | 11:AK:58:SER:N     | 2.48                     | 0.46              |
| 20:AT:35:VAL:CG1   | 20:AT:79:LEU:HD22  | 2.46                     | 0.46              |
| 22:BA:2516:A:O2'   | 22:BA:2517:C:H5'   | 2.15                     | 0.46              |
| 22:BA:2609:U:O2'   | 22:BA:2610:C:H5'   | 2.16                     | 0.46              |
| 23:BB:37:C:C5      | 23:BB:38:C:C5      | 3.04                     | 0.46              |
| 24:BC:252:THR:HG22 | 24:BC:253:LYS:N    | 2.30                     | 0.46              |
| 26:BE:155:GLU:OE2  | 26:BE:159:LEU:HD21 | 2.16                     | 0.46              |
| 27:BF:148:ARG:CG   | 27:BF:149:VAL:N    | 2.78                     | 0.46              |
| 27:BF:17:MET:HE3   | 27:BF:17:MET:HA    | 1.98                     | 0.46              |
| 30:BI:112:THR:O    | 30:BI:114:ALA:N    | 2.48                     | 0.46              |
| 34:BM:135:VAL:HG23 | 34:BM:135:VAL:O    | 2.16                     | 0.46              |
| 35:BN:31:HIS:C     | 35:BN:33:ILE:H     | 2.19                     | 0.46              |
| 35:BN:65:LEU:HD11  | 35:BN:69:ARG:HH21  | 1.78                     | 0.46              |
| 1:CA:1227:A:OP2    | 13:CM:110:LYS:HD2  | 2.15                     | 0.46              |
| 1:CA:728:A:N1      | 1:CA:729:A:C6      | 2.84                     | 0.46              |
| 1:CA:798:U:C2'     | 1:CA:799:G:O5'     | 2.64                     | 0.46              |
| 1:CA:78:A:C2       | 1:CA:92:U:O2       | 2.69                     | 0.46              |
| 1:CA:93:U:C2'      | 1:CA:94:G:H5''     | 2.46                     | 0.46              |
| 3:CC:111:LEU:HD22  | 3:CC:111:LEU:N     | 2.31                     | 0.46              |
| 1:CA:620:C:N1      | 4:CD:132:ILE:HD13  | 2.30                     | 0.46              |
| 4:CD:146:ARG:O     | 4:CD:150:LYS:HB2   | 2.16                     | 0.46              |
| 4:CD:26:ARG:CG     | 4:CD:27:ALA:N      | 2.74                     | 0.46              |
| 4:CD:58:LYS:CB     | 4:CD:200:ILE:HB    | 2.46                     | 0.46              |
| 6:CF:86:ARG:NH1    | 6:CF:86:ARG:CG     | 2.77                     | 0.46              |
| 7:CG:99:LEU:HB3    | 7:CG:103:TRP:CZ2   | 2.50                     | 0.46              |
| 1:CA:684:U:C2'     | 11:CK:40:ASN:O     | 2.64                     | 0.46              |
| 13:CM:23:TYR:O     | 13:CM:23:TYR:CD2   | 2.69                     | 0.46              |
| 52:D4:25:VAL:HB    | 52:D4:35:GLN:HB2   | 1.98                     | 0.46              |
| 22:DA:1062:G:C6    | 22:DA:1063:G:O6    | 2.69                     | 0.46              |
| 22:DA:583:G:N2     | 22:DA:1258:U:C2    | 2.84                     | 0.46              |
| 22:DA:1364:G:N7    | 45:DX:2:SER:N      | 2.64                     | 0.46              |
| 22:DA:1425:G:H2'   | 22:DA:1426:G:O4'   | 2.16                     | 0.46              |
| 22:DA:1585:C:C5    | 22:DA:1586:A:N7    | 2.84                     | 0.46              |
| 22:DA:1861:G:N1    | 22:DA:1882:U:O2    | 2.48                     | 0.46              |
| 22:DA:2499:C:C4    | 22:DA:2500:U:O4    | 2.69                     | 0.46              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:DA:2584:U:OP2  | 22:DA:2585:U:C5    | 2.68                     | 0.46              |
| 22:DA:2853:C:H2'  | 22:DA:2854:G:C8    | 2.51                     | 0.46              |
| 22:DA:2893:A:O4'  | 22:DA:2894:G:C2    | 2.68                     | 0.46              |
| 22:DA:38:A:C2     | 22:DA:442:G:O6     | 2.68                     | 0.46              |
| 22:DA:477:A:C2'   | 22:DA:478:A:O5'    | 2.63                     | 0.46              |
| 22:DA:488:G:N1    | 22:DA:491:G:OP2    | 2.49                     | 0.46              |
| 22:DA:601:C:H2'   | 22:DA:602:A:O4'    | 2.16                     | 0.46              |
| 22:DA:704:G:H1'   | 22:DA:726:G:N2     | 2.31                     | 0.46              |
| 22:DA:973:A:O4'   | 22:DA:1188:U:C6    | 2.69                     | 0.46              |
| 25:DD:177:VAL:CG2 | 25:DD:187:LEU:HD11 | 2.46                     | 0.46              |
| 28:DG:123:ALA:HB2 | 28:DG:133:LEU:HA   | 1.98                     | 0.46              |
| 28:DG:96:ALA:O    | 28:DG:128:GLN:HA   | 2.16                     | 0.46              |
| 34:DM:97:GLN:OE1  | 34:DM:97:GLN:N     | 2.49                     | 0.46              |
| 35:DN:43:GLU:HA   | 35:DN:43:GLU:OE1   | 2.15                     | 0.46              |
| 42:DU:12:ILE:HG21 | 42:DU:80:ALA:HB2   | 1.96                     | 0.46              |
| 42:DU:57:GLY:O    | 42:DU:59:VAL:HG23  | 2.16                     | 0.46              |
| 42:DU:85:PHE:N    | 42:DU:85:PHE:CD1   | 2.84                     | 0.46              |
| 1:AA:1005:A:H4'   | 1:AA:1037:C:H1'    | 1.98                     | 0.46              |
| 1:AA:1063:C:H2'   | 1:AA:1064:G:C8     | 2.51                     | 0.46              |
| 1:AA:23:C:C4      | 1:AA:24:U:C5       | 3.04                     | 0.46              |
| 1:AA:459:A:N6     | 1:AA:460:A:N6      | 2.63                     | 0.46              |
| 1:AA:730:G:H2'    | 1:AA:730:G:N3      | 2.30                     | 0.46              |
| 1:AA:850:U:H2'    | 1:AA:851:G:O5'     | 2.16                     | 0.46              |
| 1:AA:935:A:C2     | 1:AA:936:C:C2      | 3.04                     | 0.46              |
| 2:AB:149:GLY:O    | 2:AB:151:ILE:N     | 2.49                     | 0.46              |
| 2:AB:43:LEU:O     | 2:AB:46:THR:OG1    | 2.34                     | 0.46              |
| 3:AC:167:TRP:C    | 3:AC:167:TRP:CE3   | 2.90                     | 0.46              |
| 4:AD:107:PHE:CG   | 4:AD:145:ILE:HD11  | 2.50                     | 0.46              |
| 5:AE:107:ALA:HB1  | 5:AE:125:ALA:HB3   | 1.98                     | 0.46              |
| 1:AA:826:C:H5'    | 8:AH:13:ARG:CZ     | 2.46                     | 0.46              |
| 9:AI:13:LYS:O     | 9:AI:15:SER:N      | 2.44                     | 0.46              |
| 14:AN:12:LYS:O    | 14:AN:16:LEU:HG    | 2.15                     | 0.46              |
| 14:AN:41:ARG:O    | 14:AN:42:TRP:C     | 2.55                     | 0.46              |
| 16:AP:30:GLY:O    | 16:AP:31:ARG:C     | 2.54                     | 0.46              |
| 17:AQ:12:VAL:O    | 17:AQ:22:VAL:O     | 2.34                     | 0.46              |
| 22:BA:1000:A:C6   | 22:BA:1001:A:C6    | 3.04                     | 0.46              |
| 22:BA:1510:G:H2'  | 22:BA:1511:G:O4'   | 2.16                     | 0.46              |
| 22:BA:1688:U:C5'  | 22:BA:1689:A:OP1   | 2.64                     | 0.46              |
| 22:BA:1946:U:H2'  | 22:BA:1947:C:C6    | 2.51                     | 0.46              |
| 22:BA:2164:C:H3'  | 22:BA:2165:C:H5''  | 1.98                     | 0.46              |
| 22:BA:2725:A:C4   | 22:BA:2727:A:C8    | 3.04                     | 0.46              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 22:BA:422:A:C2     | 22:BA:423:A:N3    | 2.84                     | 0.46              |
| 22:BA:493:G:H2'    | 22:BA:494:G:O4'   | 2.16                     | 0.46              |
| 22:BA:5:A:H2'      | 22:BA:6:A:C8      | 2.51                     | 0.46              |
| 22:BA:790:U:O2'    | 22:BA:791:C:P     | 2.74                     | 0.46              |
| 22:BA:945:A:H4'    | 22:BA:946:C:OP2   | 2.16                     | 0.46              |
| 22:BA:1818:U:OP2   | 24:BC:156:ARG:NH1 | 2.49                     | 0.46              |
| 25:BD:104:VAL:HG23 | 25:BD:105:LYS:N   | 2.31                     | 0.46              |
| 28:BG:94:TYR:C     | 28:BG:95:ARG:HG2  | 2.36                     | 0.46              |
| 30:BI:65:ARG:NH1   | 30:BI:66:SER:OG   | 2.48                     | 0.46              |
| 33:BL:132:ARG:HG3  | 33:BL:142:ILE:CD1 | 2.46                     | 0.46              |
| 35:BN:117:ASP:O    | 35:BN:119:SER:N   | 2.49                     | 0.46              |
| 1:CA:1260:G:OP1    | 1:CA:1284:C:O2'   | 2.19                     | 0.46              |
| 1:CA:1315:U:C5     | 1:CA:1316:G:C5    | 3.04                     | 0.46              |
| 1:CA:1388:C:H2'    | 1:CA:1389:C:H6    | 1.81                     | 0.46              |
| 1:CA:139:A:O2'     | 1:CA:140:U:H5'    | 2.16                     | 0.46              |
| 1:CA:441:A:C2      | 1:CA:497:G:C6     | 3.04                     | 0.46              |
| 1:CA:71:A:C6       | 1:CA:72:A:N7      | 2.84                     | 0.46              |
| 1:CA:819:A:H4'     | 1:CA:820:U:OP2    | 2.16                     | 0.46              |
| 1:CA:9:G:H5'       | 5:CE:108:GLY:HA3  | 1.97                     | 0.46              |
| 2:CB:207:ILE:N     | 2:CB:207:ILE:HD13 | 2.30                     | 0.46              |
| 1:CA:1056:U:H4'    | 3:CC:163:ALA:HB2  | 1.98                     | 0.46              |
| 3:CC:184:TYR:CD1   | 3:CC:201:TRP:CD1  | 3.04                     | 0.46              |
| 4:CD:9:LEU:HG      | 4:CD:32:CYS:HB2   | 1.98                     | 0.46              |
| 4:CD:33:LYS:NZ     | 4:CD:33:LYS:HB2   | 2.31                     | 0.46              |
| 5:CE:104:GLY:O     | 5:CE:105:ILE:HG22 | 2.16                     | 0.46              |
| 8:CH:35:ALA:O      | 8:CH:39:VAL:HG23  | 2.16                     | 0.46              |
| 9:CI:116:VAL:HG21  | 10:CJ:62:ARG:HD3  | 1.97                     | 0.46              |
| 12:CL:18:LYS:HD2   | 12:CL:18:LYS:O    | 2.16                     | 0.46              |
| 14:CN:62:ASN:OD1   | 14:CN:73:PHE:CE1  | 2.69                     | 0.46              |
| 15:CO:37:ASN:O     | 15:CO:40:GLN:HB2  | 2.16                     | 0.46              |
| 22:DA:2885:G:N2    | 48:D0:32:LYS:HA   | 2.30                     | 0.46              |
| 22:DA:1068:G:H2'   | 22:DA:1096:A:H5'  | 1.98                     | 0.46              |
| 22:DA:1568:G:N3    | 24:DC:58:HIS:CE1  | 2.84                     | 0.46              |
| 22:DA:1652:A:H3'   | 22:DA:1653:G:C8   | 2.51                     | 0.46              |
| 22:DA:1817:G:H4'   | 24:DC:86:ASN:O    | 2.15                     | 0.46              |
| 22:DA:200:U:C6     | 22:DA:201:C:C5    | 3.04                     | 0.46              |
| 22:DA:2200:C:O2    | 22:DA:2226:C:N4   | 2.48                     | 0.46              |
| 22:DA:2439:A:H4'   | 22:DA:2440:C:H5'' | 1.98                     | 0.46              |
| 22:DA:2473:U:O2    | 22:DA:2473:U:H2'  | 2.16                     | 0.46              |
| 22:DA:1783:A:C2    | 22:DA:2588:G:O4'  | 2.68                     | 0.46              |
| 22:DA:2650:U:H2'   | 22:DA:2651:C:C6   | 2.51                     | 0.46              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:DA:523:C:H2'    | 22:DA:524:G:C8     | 2.51                     | 0.46              |
| 22:DA:528:A:C2     | 22:DA:2043:C:H4'   | 2.51                     | 0.46              |
| 24:DC:107:PRO:HD2  | 24:DC:110:LEU:HD22 | 1.98                     | 0.46              |
| 28:DG:126:PRO:C    | 28:DG:127:THR:OG1  | 2.53                     | 0.46              |
| 30:DI:76:ALA:HB2   | 30:DI:129:ILE:HG23 | 1.96                     | 0.46              |
| 30:DI:80:LEU:HA    | 30:DI:84:ALA:HB3   | 1.98                     | 0.46              |
| 37:DP:51:ARG:O     | 37:DP:57:SER:HA    | 2.16                     | 0.46              |
| 39:DR:39:LEU:C     | 39:DR:49:ILE:HG23  | 2.36                     | 0.46              |
| 1:AA:1227:A:H2'    | 1:AA:1228:C:O5'    | 2.17                     | 0.45              |
| 1:AA:1319:A:C8     | 1:AA:1323:G:C5     | 3.04                     | 0.45              |
| 1:AA:141:G:C2      | 1:AA:142:G:H1'     | 2.51                     | 0.45              |
| 1:AA:142:G:H3'     | 1:AA:143:A:H8      | 1.81                     | 0.45              |
| 1:AA:186:C:H2'     | 1:AA:187:G:O4'     | 2.15                     | 0.45              |
| 1:AA:242:G:C2      | 1:AA:245:U:C4      | 3.05                     | 0.45              |
| 1:AA:614:C:H2'     | 1:AA:615:G:O4'     | 2.15                     | 0.45              |
| 4:AD:68:LEU:CD2    | 4:AD:68:LEU:N      | 2.79                     | 0.45              |
| 9:AI:85:ARG:O      | 9:AI:88:MET:CB     | 2.64                     | 0.45              |
| 12:AL:63:VAL:HG22  | 12:AL:64:THR:N     | 2.31                     | 0.45              |
| 14:AN:28:LYS:N     | 14:AN:31:ILE:HB    | 2.32                     | 0.45              |
| 15:AO:61:SER:O     | 15:AO:65:LYS:HG3   | 2.16                     | 0.45              |
| 16:AP:77:GLU:C     | 16:AP:79:ASN:H     | 2.19                     | 0.45              |
| 20:AT:3:ASN:O      | 20:AT:4:ILE:C      | 2.54                     | 0.45              |
| 22:BA:1106:G:C2    | 22:BA:1107:G:C8    | 3.04                     | 0.45              |
| 22:BA:1665:A:H5''  | 32:BK:66:LYS:HB3   | 1.98                     | 0.45              |
| 22:BA:1936:A:H2    | 22:BA:1943:U:N3    | 2.11                     | 0.45              |
| 22:BA:1949:G:N2    | 22:BA:1958:C:C2    | 2.84                     | 0.45              |
| 22:BA:1964:G:O2'   | 22:BA:1967:C:OP2   | 2.21                     | 0.45              |
| 22:BA:2305:U:H5''  | 27:BF:131:GLY:HA3  | 1.97                     | 0.45              |
| 22:BA:868:U:C4     | 22:BA:869:G:N7     | 2.84                     | 0.45              |
| 25:BD:16:THR:O     | 25:BD:17:GLU:C     | 2.54                     | 0.45              |
| 27:BF:38:MET:HE2   | 27:BF:152:LEU:HD22 | 1.98                     | 0.45              |
| 28:BG:40:ALA:HB2   | 28:BG:58:TYR:CD2   | 2.51                     | 0.45              |
| 29:BH:90:LEU:HD21  | 29:BH:93:SER:HA    | 1.97                     | 0.45              |
| 31:BJ:81:ILE:CG2   | 31:BJ:82:GLY:N     | 2.72                     | 0.45              |
| 33:BL:122:VAL:HG21 | 33:BL:135:ILE:HD13 | 1.98                     | 0.45              |
| 35:BN:24:MET:CE    | 35:BN:44:LEU:HD13  | 2.46                     | 0.45              |
| 39:BR:39:LEU:HA    | 39:BR:49:ILE:HG21  | 1.96                     | 0.45              |
| 47:BZ:10:THR:HG23  | 47:BZ:11:ARG:HG3   | 1.99                     | 0.45              |
| 1:CA:1007:U:C2'    | 1:CA:1008:U:H5'    | 2.45                     | 0.45              |
| 1:CA:1055:A:N7     | 1:CA:1206:G:C6     | 2.84                     | 0.45              |
| 1:CA:1244:G:C6     | 1:CA:1245:C:N4     | 2.84                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CA:1392:G:O2'   | 1:CA:1393:U:H5'   | 2.15                     | 0.45              |
| 1:CA:1457:G:H2'   | 1:CA:1458:G:O4'   | 2.16                     | 0.45              |
| 1:CA:18:C:C2      | 1:CA:19:A:C8      | 3.04                     | 0.45              |
| 4:CD:42:GLY:C     | 4:CD:44:ARG:H     | 2.19                     | 0.45              |
| 8:CH:77:ARG:HD3   | 8:CH:78:VAL:N     | 2.31                     | 0.45              |
| 8:CH:89:LYS:HA    | 8:CH:92:LEU:HD13  | 1.98                     | 0.45              |
| 10:CJ:40:ILE:HG22 | 10:CJ:42:LEU:HG   | 1.96                     | 0.45              |
| 11:CK:97:ILE:HG13 | 11:CK:98:ARG:N    | 2.30                     | 0.45              |
| 13:CM:22:ILE:HD12 | 13:CM:22:ILE:N    | 2.31                     | 0.45              |
| 14:CN:48:LEU:O    | 14:CN:48:LEU:HD23 | 2.16                     | 0.45              |
| 17:CQ:14:SER:HB3  | 17:CQ:22:VAL:CG1  | 2.46                     | 0.45              |
| 21:CU:34:ARG:HE   | 21:CU:35:ARG:HB2  | 1.82                     | 0.45              |
| 49:D1:11:LEU:HB2  | 49:D1:21:TYR:HB2  | 1.98                     | 0.45              |
| 22:DA:126:A:N3    | 50:D2:18:PHE:CE2  | 2.84                     | 0.45              |
| 22:DA:1355:G:C6   | 22:DA:1377:G:C2   | 3.03                     | 0.45              |
| 22:DA:1379:U:O2   | 22:DA:1379:U:H2'  | 2.16                     | 0.45              |
| 22:DA:1459:G:C2   | 22:DA:1461:C:C2   | 3.04                     | 0.45              |
| 22:DA:170:U:N3    | 22:DA:171:U:C5    | 2.84                     | 0.45              |
| 22:DA:118:A:N3    | 22:DA:178:G:H1'   | 2.31                     | 0.45              |
| 22:DA:1651:G:N2   | 22:DA:2007:U:C2   | 2.84                     | 0.45              |
| 22:DA:2291:U:H2'  | 22:DA:2292:U:C6   | 2.51                     | 0.45              |
| 22:DA:2373:G:C6   | 22:DA:2381:A:N1   | 2.84                     | 0.45              |
| 22:DA:2725:A:C5   | 22:DA:2727:A:C8   | 3.04                     | 0.45              |
| 22:DA:2734:A:N7   | 22:DA:2735:G:N7   | 2.64                     | 0.45              |
| 22:DA:449:A:N7    | 22:DA:450:G:N7    | 2.64                     | 0.45              |
| 22:DA:609:A:C5    | 22:DA:610:C:O2    | 2.70                     | 0.45              |
| 22:DA:609:A:H2'   | 22:DA:610:C:O4'   | 2.16                     | 0.45              |
| 22:DA:712:G:N2    | 22:DA:720:U:H1'   | 2.31                     | 0.45              |
| 22:DA:982:C:H5'   | 22:DA:983:A:OP1   | 2.15                     | 0.45              |
| 26:DE:40:ARG:NH2  | 26:DE:92:HIS:CE1  | 2.85                     | 0.45              |
| 27:DF:111:ILE:HB  | 27:DF:114:PHE:HB2 | 1.97                     | 0.45              |
| 29:DH:112:LYS:HG2 | 29:DH:113:SER:N   | 2.32                     | 0.45              |
| 29:DH:39:ALA:O    | 29:DH:41:LYS:N    | 2.47                     | 0.45              |
| 37:DP:103:ARG:HB3 | 37:DP:108:ALA:CB  | 2.46                     | 0.45              |
| 41:DT:32:LEU:O    | 41:DT:32:LEU:HD12 | 2.16                     | 0.45              |
| 46:DY:14:LEU:HD21 | 46:DY:57:LEU:HD21 | 1.98                     | 0.45              |
| 47:DZ:3:LYS:CD    | 47:DZ:3:LYS:N     | 2.78                     | 0.45              |
| 1:AA:1024:G:C2'   | 1:AA:1025:U:O5'   | 2.65                     | 0.45              |
| 1:AA:1144:G:N1    | 1:AA:1145:A:H2    | 2.14                     | 0.45              |
| 1:AA:181:A:H1'    | 1:AA:194:C:N4     | 2.31                     | 0.45              |
| 1:AA:427:U:C4     | 1:AA:428:G:C6     | 3.04                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:AB:72:THR:O     | 2:AB:73:LYS:HG2   | 2.16                     | 0.45              |
| 2:AB:84:ALA:O     | 2:AB:89:GLN:HB2   | 2.16                     | 0.45              |
| 8:AH:42:GLU:N     | 8:AH:42:GLU:OE1   | 2.49                     | 0.45              |
| 9:AI:50:GLN:N     | 9:AI:51:PRO:HD2   | 2.31                     | 0.45              |
| 10:AJ:17:LEU:HD23 | 10:AJ:18:ILE:N    | 2.32                     | 0.45              |
| 12:AL:110:ARG:NH1 | 12:AL:113:ALA:HB3 | 2.30                     | 0.45              |
| 13:AM:29:ARG:NH2  | 13:AM:63:PHE:HB2  | 2.31                     | 0.45              |
| 16:AP:67:ILE:HG23 | 16:AP:71:VAL:CG1  | 2.46                     | 0.45              |
| 17:AQ:10:GLY:HA3  | 17:AQ:24:ALA:O    | 2.17                     | 0.45              |
| 21:AU:19:PHE:O    | 21:AU:22:SER:HB3  | 2.16                     | 0.45              |
| 22:BA:1161:C:H1'  | 39:BR:8:GLY:O     | 2.17                     | 0.45              |
| 22:BA:1333:G:C2   | 22:BA:1334:G:C8   | 3.04                     | 0.45              |
| 22:BA:1385:A:N3   | 22:BA:1386:C:C6   | 2.84                     | 0.45              |
| 22:BA:1570:A:C6   | 22:BA:1571:A:C6   | 3.05                     | 0.45              |
| 22:BA:2293:G:H2'  | 22:BA:2294:G:O4'  | 2.17                     | 0.45              |
| 22:BA:536:G:C6    | 22:BA:537:G:C4    | 3.04                     | 0.45              |
| 22:BA:54:G:C5     | 22:BA:55:G:C8     | 3.05                     | 0.45              |
| 22:BA:784:G:H5'   | 24:BC:226:ASN:OD1 | 2.16                     | 0.45              |
| 24:BC:77:VAL:HA   | 24:BC:114:ASP:O   | 2.16                     | 0.45              |
| 26:BE:79:ARG:O    | 26:BE:80:SER:CB   | 2.63                     | 0.45              |
| 29:BH:79:THR:HG23 | 29:BH:147:VAL:HB  | 1.98                     | 0.45              |
| 30:BI:105:GLN:O   | 30:BI:106:LEU:CB  | 2.65                     | 0.45              |
| 30:BI:50:GLU:OE2  | 30:BI:52:GLY:N    | 2.50                     | 0.45              |
| 30:BI:75:PRO:O    | 30:BI:78:VAL:HG22 | 2.16                     | 0.45              |
| 1:AA:1423:G:P     | 32:BK:49:ARG:HH22 | 2.39                     | 0.45              |
| 35:BN:38:LEU:HB3  | 35:BN:39:PRO:HD3  | 1.99                     | 0.45              |
| 41:BT:57:VAL:HG22 | 41:BT:58:VAL:N    | 2.30                     | 0.45              |
| 42:BU:85:PHE:N    | 42:BU:85:PHE:CD1  | 2.83                     | 0.45              |
| 1:CA:968:A:C8     | 1:CA:1062:U:H4'   | 2.51                     | 0.45              |
| 1:CA:1073:U:H5'   | 1:CA:1074:G:OP2   | 2.17                     | 0.45              |
| 1:CA:124:C:N3     | 1:CA:125:U:C4     | 2.84                     | 0.45              |
| 1:CA:1310:G:N2    | 1:CA:1328:C:O2    | 2.49                     | 0.45              |
| 1:CA:1426:G:C4    | 1:CA:1475:G:C2    | 3.05                     | 0.45              |
| 1:CA:442:G:C6     | 1:CA:443:C:C4     | 3.04                     | 0.45              |
| 1:CA:510:A:H5''   | 1:CA:511:C:P      | 2.56                     | 0.45              |
| 1:CA:525:C:N4     | 1:CA:526:C:N4     | 2.63                     | 0.45              |
| 1:CA:701:U:H4'    | 1:CA:703:G:C8     | 2.51                     | 0.45              |
| 1:CA:669:G:N2     | 1:CA:738:C:O2     | 2.48                     | 0.45              |
| 1:CA:756:C:C2'    | 1:CA:757:U:H5'    | 2.46                     | 0.45              |
| 1:CA:81:A:H2'     | 1:CA:82:G:C8      | 2.51                     | 0.45              |
| 1:CA:992:U:O4'    | 1:CA:993:G:C2     | 2.68                     | 0.45              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:CB:186:ILE:HA   | 2:CB:200:ILE:O     | 2.16                     | 0.45              |
| 2:CB:90:PHE:HB3   | 2:CB:150:GLY:O     | 2.16                     | 0.45              |
| 4:CD:74:ASN:HA    | 4:CD:77:LYS:HB2    | 1.98                     | 0.45              |
| 4:CD:78:GLU:CG    | 4:CD:93:LEU:HD11   | 2.46                     | 0.45              |
| 1:CA:429:U:H3'    | 4:CD:9:LEU:HD23    | 1.98                     | 0.45              |
| 5:CE:150:PRO:HA   | 8:CH:99:LEU:HD21   | 1.98                     | 0.45              |
| 6:CF:51:ILE:CG1   | 6:CF:51:ILE:O      | 2.63                     | 0.45              |
| 12:CL:9:ARG:HB2   | 12:CL:9:ARG:CZ     | 2.46                     | 0.45              |
| 1:CA:952:U:O4     | 13:CM:103:LYS:HD3  | 2.15                     | 0.45              |
| 13:CM:96:PRO:CB   | 13:CM:100:GLN:OE1  | 2.65                     | 0.45              |
| 15:CO:11:ILE:O    | 15:CO:14:GLU:HB2   | 2.16                     | 0.45              |
| 17:CQ:13:VAL:HG13 | 17:CQ:22:VAL:HG13  | 1.98                     | 0.45              |
| 17:CQ:14:SER:OG   | 17:CQ:22:VAL:HG12  | 2.16                     | 0.45              |
| 20:CT:54:MET:HE2  | 20:CT:58:VAL:CG2   | 2.47                     | 0.45              |
| 21:CU:29:LEU:C    | 21:CU:29:LEU:HD23  | 2.37                     | 0.45              |
| 33:DL:62:PRO:HG3  | 51:D3:26:HIS:O     | 2.17                     | 0.45              |
| 22:DA:1066:U:C2'  | 22:DA:1067:A:OP1   | 2.64                     | 0.45              |
| 22:DA:1345:C:H5'  | 22:DA:1396:U:C4    | 2.51                     | 0.45              |
| 22:DA:142:A:C6    | 22:DA:143:C:N4     | 2.84                     | 0.45              |
| 22:DA:1949:G:C6   | 22:DA:1950:G:C6    | 3.04                     | 0.45              |
| 22:DA:2051:A:C2   | 22:DA:2052:A:N6    | 2.84                     | 0.45              |
| 22:DA:2163:A:H2'  | 22:DA:2164:C:H4'   | 1.98                     | 0.45              |
| 22:DA:2361:G:H2'  | 22:DA:2362:C:O4'   | 2.17                     | 0.45              |
| 22:DA:2571:U:N3   | 22:DA:2574:G:C8    | 2.85                     | 0.45              |
| 22:DA:2643:G:C2'  | 22:DA:2644:G:H5'   | 2.47                     | 0.45              |
| 22:DA:609:A:N7    | 22:DA:610:C:C2     | 2.85                     | 0.45              |
| 22:DA:58:G:C2     | 22:DA:70:G:C2      | 3.04                     | 0.45              |
| 23:DB:20:G:C2     | 23:DB:64:G:C2      | 3.05                     | 0.45              |
| 23:DB:84:G:N2     | 23:DB:93:C:O2      | 2.49                     | 0.45              |
| 24:DC:120:VAL:O   | 24:DC:120:VAL:HG12 | 2.15                     | 0.45              |
| 24:DC:148:PRO:CD  | 24:DC:185:GLU:OE2  | 2.64                     | 0.45              |
| 1:AA:1027:C:C2    | 1:AA:1034:G:O6     | 2.69                     | 0.45              |
| 1:AA:1086:U:O2'   | 1:AA:1087:G:H5'    | 2.17                     | 0.45              |
| 1:AA:29:U:H5'     | 1:AA:296:U:OP1     | 2.16                     | 0.45              |
| 1:AA:55:A:C6      | 1:AA:56:U:C2       | 3.05                     | 0.45              |
| 1:AA:597:G:C2     | 1:AA:644:U:O2      | 2.69                     | 0.45              |
| 1:AA:72:A:C2'     | 1:AA:73:C:H5'      | 2.46                     | 0.45              |
| 1:AA:785:G:N2     | 1:AA:798:U:C2      | 2.83                     | 0.45              |
| 2:AB:21:ARG:HA    | 2:AB:21:ARG:NH1    | 2.30                     | 0.45              |
| 3:AC:22:TRP:CD1   | 3:AC:59:ARG:CD     | 2.99                     | 0.45              |
| 4:AD:3:ARG:CZ     | 4:AD:115:ARG:CD    | 2.92                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:AH:7:ILE:HD12   | 8:AH:7:ILE:N      | 2.31                     | 0.45              |
| 8:AH:79:SER:HA    | 8:AH:85:ILE:HG12  | 1.98                     | 0.45              |
| 9:AI:22:LYS:HD2   | 9:AI:23:PRO:O     | 2.17                     | 0.45              |
| 9:AI:57:MET:CG    | 9:AI:58:VAL:N     | 2.79                     | 0.45              |
| 10:AJ:44:THR:HG22 | 10:AJ:70:HIS:HA   | 1.99                     | 0.45              |
| 13:AM:51:GLY:O    | 13:AM:55:THR:HG23 | 2.17                     | 0.45              |
| 20:AT:67:ILE:CG1  | 20:AT:71:LYS:HG2  | 2.45                     | 0.45              |
| 21:AU:11:PRO:O    | 21:AU:12:PHE:CG   | 2.69                     | 0.45              |
| 21:AU:37:PHE:HA   | 21:AU:40:LYS:HE3  | 1.99                     | 0.45              |
| 53:B5:79:ALA:CB   | 53:B5:83:LYS:HB2  | 2.46                     | 0.45              |
| 22:BA:1056:G:C2   | 22:BA:1102:C:C5   | 3.04                     | 0.45              |
| 22:BA:1402:U:C2'  | 22:BA:1403:A:O5'  | 2.64                     | 0.45              |
| 22:BA:1768:C:N3   | 22:BA:1769:U:C5   | 2.84                     | 0.45              |
| 22:BA:1796:U:H2'  | 22:BA:1797:G:C8   | 2.51                     | 0.45              |
| 22:BA:2714:G:H2'  | 22:BA:2715:C:H5'  | 1.98                     | 0.45              |
| 22:BA:271:G:C5    | 22:BA:367:G:C2    | 3.04                     | 0.45              |
| 22:BA:360:U:C4    | 22:BA:361:G:C6    | 3.04                     | 0.45              |
| 22:BA:365:U:H2'   | 22:BA:366:C:C6    | 2.51                     | 0.45              |
| 22:BA:593:U:H2'   | 22:BA:594:U:C6    | 2.51                     | 0.45              |
| 22:BA:979:A:H2'   | 22:BA:982:C:H42   | 1.82                     | 0.45              |
| 25:BD:166:GLY:O   | 25:BD:167:ASN:HB3 | 2.16                     | 0.45              |
| 22:BA:675:A:OP1   | 26:BE:58:LYS:HE3  | 2.16                     | 0.45              |
| 29:BH:94:ILE:HG23 | 29:BH:98:ASP:CB   | 2.47                     | 0.45              |
| 22:BA:1139:G:O3'  | 31:BJ:26:GLY:HA3  | 2.16                     | 0.45              |
| 35:BN:22:ARG:HG3  | 35:BN:70:THR:H    | 1.80                     | 0.45              |
| 35:BN:78:LYS:C    | 35:BN:79:LEU:O    | 2.49                     | 0.45              |
| 1:CA:1015:G:H2'   | 1:CA:1016:A:O4'   | 2.17                     | 0.45              |
| 1:CA:1137:C:H1'   | 1:CA:1138:G:N2    | 2.31                     | 0.45              |
| 1:CA:22:G:O2'     | 1:CA:913:A:N1     | 2.43                     | 0.45              |
| 5:CE:126:LYS:HE3  | 5:CE:126:LYS:HA   | 1.97                     | 0.45              |
| 5:CE:154:ALA:C    | 5:CE:156:LYS:N    | 2.70                     | 0.45              |
| 5:CE:95:PHE:CG    | 5:CE:96:MET:N     | 2.84                     | 0.45              |
| 5:CE:96:MET:CE    | 5:CE:111:MET:HE3  | 2.46                     | 0.45              |
| 12:CL:57:LEU:O    | 12:CL:58:THR:C    | 2.54                     | 0.45              |
| 14:CN:80:SER:O    | 14:CN:81:ARG:C    | 2.55                     | 0.45              |
| 22:DA:104:A:C8    | 22:DA:105:C:C4    | 3.04                     | 0.45              |
| 22:DA:1361:G:C5   | 22:DA:1362:C:C5   | 3.04                     | 0.45              |
| 22:DA:1649:G:N1   | 22:DA:2009:A:C6   | 2.84                     | 0.45              |
| 22:DA:1722:A:C2   | 22:DA:1739:A:H1'  | 2.51                     | 0.45              |
| 22:DA:1926:U:H2'  | 22:DA:1928:A:N7   | 2.31                     | 0.45              |
| 22:DA:195:A:C4    | 22:DA:198:C:N4    | 2.84                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:DA:2043:C:C2   | 22:DA:2044:C:C5   | 3.05                     | 0.45              |
| 22:DA:2281:A:C2'  | 22:DA:2282:G:H5'  | 2.47                     | 0.45              |
| 22:DA:2347:C:C2   | 22:DA:2371:G:N2   | 2.84                     | 0.45              |
| 22:DA:2283:C:N3   | 22:DA:2389:G:C2   | 2.84                     | 0.45              |
| 22:DA:2405:G:N2   | 22:DA:2411:A:C8   | 2.83                     | 0.45              |
| 22:DA:2532:G:N2   | 22:DA:2663:G:O2'  | 2.50                     | 0.45              |
| 22:DA:2694:G:C4   | 22:DA:2695:U:C6   | 3.04                     | 0.45              |
| 22:DA:2747:G:C2   | 22:DA:2756:U:C5   | 3.04                     | 0.45              |
| 22:DA:2817:U:O2   | 22:DA:2836:U:H1'  | 2.15                     | 0.45              |
| 22:DA:617:G:H2'   | 22:DA:618:G:O4'   | 2.16                     | 0.45              |
| 22:DA:647:G:C6    | 22:DA:648:G:C5    | 3.04                     | 0.45              |
| 22:DA:752:A:O2'   | 22:DA:753:A:P     | 2.74                     | 0.45              |
| 22:DA:7:G:H2'     | 22:DA:8:C:O4'     | 2.17                     | 0.45              |
| 22:DA:806:C:H2'   | 22:DA:807:U:C6    | 2.50                     | 0.45              |
| 23:DB:50:A:H2'    | 23:DB:51:G:O4'    | 2.16                     | 0.45              |
| 29:DH:34:GLY:O    | 29:DH:35:LYS:CD   | 2.65                     | 0.45              |
| 33:DL:37:GLY:O    | 33:DL:40:SER:OG   | 2.34                     | 0.45              |
| 41:DT:49:LYS:HD3  | 41:DT:49:LYS:N    | 2.31                     | 0.45              |
| 41:DT:67:VAL:HG12 | 41:DT:68:LYS:N    | 2.32                     | 0.45              |
| 1:AA:1202:U:C5    | 1:AA:1203:C:C5    | 3.04                     | 0.45              |
| 2:AB:33:GLY:HA3   | 2:AB:40:ILE:H     | 1.80                     | 0.45              |
| 3:AC:88:ARG:HG3   | 3:AC:99:ALA:O     | 2.15                     | 0.45              |
| 6:AF:8:PHE:CZ     | 6:AF:60:VAL:HB    | 2.52                     | 0.45              |
| 1:AA:933:G:OP2    | 7:AG:3:ARG:HB3    | 2.16                     | 0.45              |
| 13:AM:48:LEU:C    | 13:AM:48:LEU:HD23 | 2.37                     | 0.45              |
| 13:AM:85:CYS:SG   | 13:AM:87:ARG:HG3  | 2.56                     | 0.45              |
| 1:AA:1048:G:OP1   | 14:AN:3:LYS:HA    | 2.15                     | 0.45              |
| 17:AQ:59:VAL:HG23 | 17:AQ:77:ARG:O    | 2.17                     | 0.45              |
| 20:AT:7:ALA:HB1   | 20:AT:10:ARG:HB2  | 1.98                     | 0.45              |
| 22:BA:1045:C:H3'  | 22:BA:1046:A:C5'  | 2.45                     | 0.45              |
| 22:BA:1084:A:HO2' | 22:BA:1105:U:HO2' | 1.64                     | 0.45              |
| 22:BA:1098:A:H5'  | 22:BA:1099:G:OP2  | 2.16                     | 0.45              |
| 22:BA:1153:C:N4   | 22:BA:1154:G:C6   | 2.84                     | 0.45              |
| 22:BA:1228:G:H2'  | 22:BA:1229:C:C6   | 2.52                     | 0.45              |
| 22:BA:1366:A:C2   | 22:BA:1367:A:H1'  | 2.51                     | 0.45              |
| 22:BA:1385:A:H1'  | 22:BA:1386:C:H6   | 1.75                     | 0.45              |
| 22:BA:1385:A:C2   | 22:BA:1386:C:C2   | 3.05                     | 0.45              |
| 22:BA:1570:A:H2'  | 22:BA:1571:A:C8   | 2.51                     | 0.45              |
| 22:BA:1832:C:C4   | 22:BA:1833:C:C6   | 3.05                     | 0.45              |
| 22:BA:1887:C:C2'  | 22:BA:1888:G:O5'  | 2.64                     | 0.45              |
| 22:BA:1917:U:O4   | 22:BA:1918:A:C6   | 2.69                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:BA:2575:C:O2'   | 25:BD:145:SER:HB2  | 2.16                     | 0.45              |
| 22:BA:19:A:C2      | 22:BA:522:A:C2     | 3.04                     | 0.45              |
| 22:BA:581:C:H2'    | 22:BA:582:A:C8     | 2.51                     | 0.45              |
| 23:BB:65:U:O4      | 23:BB:108:A:H1'    | 2.17                     | 0.45              |
| 27:BF:111:ILE:O    | 27:BF:114:PHE:HB2  | 2.17                     | 0.45              |
| 27:BF:43:ALA:O     | 27:BF:46:ASP:C     | 2.55                     | 0.45              |
| 28:BG:127:THR:HG22 | 28:BG:128:GLN:N    | 2.32                     | 0.45              |
| 30:BI:97:LYS:HG3   | 30:BI:139:VAL:HG22 | 1.95                     | 0.45              |
| 31:BJ:77:HIS:CD2   | 31:BJ:79:GLY:H     | 2.34                     | 0.45              |
| 33:BL:49:GLY:O     | 33:BL:51:GLU:HG3   | 2.16                     | 0.45              |
| 33:BL:77:ILE:CD1   | 33:BL:95:LEU:HD13  | 2.47                     | 0.45              |
| 34:BM:24:THR:CG2   | 34:BM:24:THR:O     | 2.61                     | 0.45              |
| 40:BS:84:ARG:HB2   | 40:BS:96:ILE:CD1   | 2.46                     | 0.45              |
| 1:CA:1088:G:C6     | 1:CA:1089:G:N7     | 2.84                     | 0.45              |
| 1:CA:1134:G:H2'    | 1:CA:1135:U:O4'    | 2.16                     | 0.45              |
| 1:CA:1491:G:C5     | 1:CA:1492:A:C6     | 3.04                     | 0.45              |
| 1:CA:186:C:O2'     | 1:CA:187:G:H5'     | 2.16                     | 0.45              |
| 1:CA:569:C:H1'     | 1:CA:574:A:C4      | 2.51                     | 0.45              |
| 1:CA:68:G:C6       | 1:CA:69:G:H1'      | 2.52                     | 0.45              |
| 1:CA:784:A:H2'     | 1:CA:785:G:O4'     | 2.15                     | 0.45              |
| 1:CA:892:A:C6      | 1:CA:893:C:C4      | 3.04                     | 0.45              |
| 5:CE:99:ALA:HB2    | 5:CE:124:LEU:HG    | 1.99                     | 0.45              |
| 1:CA:1297:G:HO2'   | 7:CG:114:LYS:HZ3   | 1.54                     | 0.45              |
| 7:CG:53:ARG:NH2    | 7:CG:125:SER:OG    | 2.49                     | 0.45              |
| 8:CH:64:LYS:HE2    | 8:CH:71:VAL:HG21   | 1.98                     | 0.45              |
| 9:CI:19:VAL:HG22   | 9:CI:65:ILE:HG22   | 1.97                     | 0.45              |
| 9:CI:88:MET:HB2    | 9:CI:92:GLU:CD     | 2.37                     | 0.45              |
| 13:CM:18:ALA:CB    | 13:CM:45:ILE:HD11  | 2.47                     | 0.45              |
| 13:CM:27:LYS:O     | 13:CM:27:LYS:HD2   | 2.17                     | 0.45              |
| 16:CP:19:VAL:HG12  | 16:CP:37:GLY:C     | 2.36                     | 0.45              |
| 17:CQ:10:GLY:HA3   | 17:CQ:25:ILE:HD13  | 1.99                     | 0.45              |
| 21:CU:14:VAL:O     | 21:CU:16:LEU:CD1   | 2.65                     | 0.45              |
| 11:CK:127:ARG:HB2  | 21:CU:34:ARG:NH1   | 2.31                     | 0.45              |
| 50:D2:1:MET:O      | 50:D2:2:LYS:C      | 2.54                     | 0.45              |
| 22:DA:1036:G:C6    | 22:DA:1120:G:C5    | 3.05                     | 0.45              |
| 22:DA:1263:U:O4    | 40:DS:95:ARG:NH1   | 2.49                     | 0.45              |
| 22:DA:1464:G:N1    | 22:DA:1465:G:C5    | 2.84                     | 0.45              |
| 22:DA:155:A:H2'    | 22:DA:156:A:C8     | 2.50                     | 0.45              |
| 22:DA:14:A:H5''    | 22:DA:15:G:OP2     | 2.16                     | 0.45              |
| 22:DA:1858:A:N1    | 22:DA:1859:U:C2    | 2.84                     | 0.45              |
| 22:DA:2199:A:C5    | 22:DA:2200:C:C2    | 3.05                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:DA:2204:G:C4   | 22:DA:2205:A:C8   | 3.04                     | 0.45              |
| 22:DA:2344:U:H4'  | 22:DA:2345:G:OP1  | 2.16                     | 0.45              |
| 22:DA:236:C:H2'   | 22:DA:237:C:H6    | 1.82                     | 0.45              |
| 22:DA:263:G:N2    | 22:DA:264:C:H1'   | 2.32                     | 0.45              |
| 22:DA:2803:G:N2   | 22:DA:2804:U:C2   | 2.85                     | 0.45              |
| 22:DA:2870:C:H5'' | 35:DN:65:LEU:CD2  | 2.45                     | 0.45              |
| 22:DA:322:A:O4'   | 22:DA:340:A:H1'   | 2.17                     | 0.45              |
| 22:DA:372:G:P     | 45:DX:62:LYS:NZ   | 2.89                     | 0.45              |
| 22:DA:419:U:C2    | 22:DA:420:C:C6    | 3.04                     | 0.45              |
| 22:DA:663:G:C6    | 22:DA:664:G:C5    | 3.05                     | 0.45              |
| 22:DA:696:G:C6    | 22:DA:767:U:O2    | 2.70                     | 0.45              |
| 22:DA:902:C:H2'   | 22:DA:903:C:C6    | 2.51                     | 0.45              |
| 24:DC:171:TYR:CD2 | 24:DC:185:GLU:HA  | 2.51                     | 0.45              |
| 26:DE:23:PHE:CD1  | 26:DE:111:GLU:HG3 | 2.51                     | 0.45              |
| 35:DN:71:ARG:HG2  | 35:DN:71:ARG:HH21 | 1.80                     | 0.45              |
| 22:DA:1250:G:H5'  | 38:DQ:6:ARG:HD3   | 1.99                     | 0.45              |
| 43:DV:44:HIS:O    | 43:DV:45:ASP:C    | 2.54                     | 0.45              |
| 1:AA:1034:G:C6    | 1:AA:1035:A:C2    | 3.04                     | 0.45              |
| 1:AA:1122:U:C4    | 1:AA:1123:U:C5    | 3.05                     | 0.45              |
| 1:AA:129:A:H1'    | 1:AA:130:A:C8     | 2.51                     | 0.45              |
| 1:AA:1406:U:C2'   | 1:AA:1407:C:H5'   | 2.46                     | 0.45              |
| 1:AA:184:G:C6     | 1:AA:185:U:C4     | 3.04                     | 0.45              |
| 1:AA:21:G:N2      | 1:AA:22:G:C6      | 2.85                     | 0.45              |
| 1:AA:221:C:O2     | 1:AA:222:C:C6     | 2.69                     | 0.45              |
| 1:AA:374:A:C6     | 1:AA:375:U:C4     | 3.05                     | 0.45              |
| 1:AA:972:C:H4'    | 10:AJ:59:LYS:HE3  | 1.98                     | 0.45              |
| 2:AB:57:LEU:CD1   | 2:AB:221:VAL:HG22 | 2.46                     | 0.45              |
| 3:AC:16:LYS:HG3   | 3:AC:17:PRO:HD2   | 1.99                     | 0.45              |
| 4:AD:58:LYS:HG2   | 4:AD:203:LEU:HD22 | 1.97                     | 0.45              |
| 6:AF:46:GLN:HA    | 6:AF:56:LYS:HA    | 1.99                     | 0.45              |
| 8:AH:41:LYS:O     | 8:AH:44:GLY:N     | 2.49                     | 0.45              |
| 10:AJ:80:THR:C    | 10:AJ:82:LYS:N    | 2.67                     | 0.45              |
| 17:AQ:48:ASP:OD2  | 17:AQ:51:ASN:HA   | 2.17                     | 0.45              |
| 53:B5:172:ILE:O   | 53:B5:173:HIS:CB  | 2.64                     | 0.45              |
| 22:BA:1109:C:C4   | 22:BA:1110:G:C6   | 3.05                     | 0.45              |
| 22:BA:1277:G:H5'  | 35:BN:20:MET:HE2  | 1.98                     | 0.45              |
| 22:BA:1374:G:O2'  | 22:BA:1375:U:H5'  | 2.16                     | 0.45              |
| 22:BA:1806:C:H2'  | 22:BA:1807:G:O5'  | 2.16                     | 0.45              |
| 22:BA:686:U:C4'   | 22:BA:687:C:OP2   | 2.61                     | 0.45              |
| 30:BI:97:LYS:HB3  | 30:BI:139:VAL:CG2 | 2.47                     | 0.45              |
| 35:BN:67:PHE:CE2  | 35:BN:71:ARG:NH1  | 2.84                     | 0.45              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 39:BR:29:THR:O     | 39:BR:30:GLY:C    | 2.54                     | 0.45              |
| 1:CA:1006:G:OP1    | 1:CA:1038:C:H5''  | 2.16                     | 0.45              |
| 1:CA:1053:G:N7     | 1:CA:1200:C:C5'   | 2.79                     | 0.45              |
| 1:CA:25:C:H2'      | 1:CA:26:A:C8      | 2.51                     | 0.45              |
| 1:CA:289:G:C2      | 1:CA:290:C:C5     | 3.05                     | 0.45              |
| 1:CA:517:G:H4'     | 1:CA:519:C:C2     | 2.52                     | 0.45              |
| 3:CC:172:ARG:C     | 3:CC:174:PRO:HD3  | 2.36                     | 0.45              |
| 5:CE:102:GLY:C     | 5:CE:104:GLY:N    | 2.69                     | 0.45              |
| 5:CE:15:LEU:C      | 5:CE:15:LEU:HD12  | 2.37                     | 0.45              |
| 6:CF:6:ILE:HG22    | 6:CF:7:VAL:N      | 2.31                     | 0.45              |
| 1:CA:1377:A:C5     | 7:CG:7:ILE:HD12   | 2.51                     | 0.45              |
| 10:CJ:74:VAL:HG12  | 10:CJ:75:ASP:N    | 2.30                     | 0.45              |
| 12:CL:107:VAL:HG23 | 12:CL:117:TYR:HB3 | 1.97                     | 0.45              |
| 3:CC:20:SER:HB2    | 14:CN:92:GLU:O    | 2.17                     | 0.45              |
| 20:CT:9:LYS:O      | 20:CT:12:ILE:HG12 | 2.16                     | 0.45              |
| 20:CT:69:LYS:O     | 20:CT:71:LYS:N    | 2.49                     | 0.45              |
| 22:DA:1260:A:N6    | 57:DA:3277:HOH:O  | 2.50                     | 0.45              |
| 22:DA:1398:C:H2'   | 22:DA:1399:C:O5'  | 2.17                     | 0.45              |
| 22:DA:1437:C:N4    | 22:DA:1438:U:O4   | 2.50                     | 0.45              |
| 22:DA:1645:G:H4'   | 22:DA:1646:C:C5   | 2.51                     | 0.45              |
| 22:DA:1740:G:H2'   | 22:DA:1741:C:C6   | 2.52                     | 0.45              |
| 22:DA:1817:G:O2'   | 22:DA:1818:U:H5'  | 2.16                     | 0.45              |
| 1:CA:1418:A:O4'    | 22:DA:1959:G:H4'  | 2.16                     | 0.45              |
| 22:DA:2306:C:OP2   | 22:DA:2307:G:C2'  | 2.64                     | 0.45              |
| 22:DA:2332:C:H4'   | 22:DA:2336:A:N6   | 2.31                     | 0.45              |
| 22:DA:2799:A:C6    | 22:DA:2801:G:C4   | 3.05                     | 0.45              |
| 22:DA:333:G:C6     | 22:DA:334:C:C5    | 3.05                     | 0.45              |
| 22:DA:349:U:H2'    | 22:DA:350:G:H8    | 1.81                     | 0.45              |
| 22:DA:467:G:C2     | 22:DA:468:G:C8    | 3.05                     | 0.45              |
| 22:DA:498:G:N3     | 22:DA:499:U:C6    | 2.85                     | 0.45              |
| 22:DA:611:C:H2'    | 22:DA:612:G:O4'   | 2.16                     | 0.45              |
| 22:DA:595:C:O2     | 22:DA:663:G:C2    | 2.69                     | 0.45              |
| 22:DA:466:A:C2     | 22:DA:796:C:O4'   | 2.70                     | 0.45              |
| 27:DF:9:LYS:O      | 27:DF:13:VAL:CG2  | 2.64                     | 0.45              |
| 29:DH:147:VAL:HG12 | 29:DH:148:ALA:N   | 2.32                     | 0.45              |
| 22:DA:1250:G:H5'   | 38:DQ:6:ARG:CD    | 2.47                     | 0.45              |
| 39:DR:39:LEU:O     | 39:DR:49:ILE:HG23 | 2.16                     | 0.45              |
| 41:DT:20:ALA:O     | 41:DT:24:MET:SD   | 2.74                     | 0.45              |
| 41:DT:48:GLN:HB2   | 41:DT:49:LYS:CE   | 2.47                     | 0.45              |
| 22:DA:483:A:C1'    | 42:DU:45:HIS:HB2  | 2.47                     | 0.45              |
| 42:DU:61:LYS:HD2   | 42:DU:61:LYS:HA   | 1.82                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 46:DY:18:LEU:O     | 46:DY:22:LEU:CB    | 2.63                     | 0.45              |
| 1:AA:113:G:O2'     | 1:AA:114:U:H5'     | 2.17                     | 0.45              |
| 1:AA:1054:C:C5     | 1:AA:1196:A:H2'    | 2.51                     | 0.45              |
| 1:AA:1335:U:H5'    | 1:AA:1336:C:O5'    | 2.17                     | 0.45              |
| 1:AA:1441:A:C2'    | 1:AA:1442:G:O5'    | 2.64                     | 0.45              |
| 1:AA:654:G:H2'     | 1:AA:655:A:H5'     | 1.98                     | 0.45              |
| 1:AA:657:U:O2      | 15:AO:22:THR:HG22  | 2.16                     | 0.45              |
| 1:AA:652:U:C2      | 1:AA:752:G:N2      | 2.85                     | 0.45              |
| 3:AC:14:ILE:O      | 3:AC:15:VAL:HG22   | 2.16                     | 0.45              |
| 1:AA:1108:G:H5'    | 3:AC:176:HIS:CE1   | 2.51                     | 0.45              |
| 3:AC:23:PHE:CE1    | 10:AJ:13:PHE:CE2   | 3.04                     | 0.45              |
| 4:AD:122:ALA:C     | 4:AD:123:ILE:HG23  | 2.36                     | 0.45              |
| 4:AD:27:ALA:O      | 4:AD:28:ILE:C      | 2.55                     | 0.45              |
| 5:AE:151:GLU:HG2   | 5:AE:152:MET:H     | 1.82                     | 0.45              |
| 1:AA:1368:A:OP2    | 9:AI:114:LYS:HD2   | 2.17                     | 0.45              |
| 10:AJ:83:THR:HA    | 10:AJ:86:ALA:HB3   | 1.98                     | 0.45              |
| 11:AK:108:THR:HG22 | 11:AK:109:ASN:ND2  | 2.31                     | 0.45              |
| 11:AK:35:THR:OG1   | 11:AK:40:ASN:N     | 2.50                     | 0.45              |
| 1:AA:1308:U:OP1    | 13:AM:96:PRO:HA    | 2.16                     | 0.45              |
| 17:AQ:47:HIS:CB    | 17:AQ:67:LEU:HD23  | 2.47                     | 0.45              |
| 49:B1:10:LYS:HE3   | 49:B1:53:LYS:NZ    | 2.32                     | 0.45              |
| 53:B5:64:SER:O     | 53:B5:65:LEU:CB    | 2.65                     | 0.45              |
| 53:B5:78:ILE:HG23  | 53:B5:78:ILE:O     | 2.17                     | 0.45              |
| 22:BA:1857:G:C4    | 22:BA:1884:G:C2    | 3.04                     | 0.45              |
| 22:BA:1935:G:C6    | 22:BA:1962:C:C5    | 3.04                     | 0.45              |
| 22:BA:250:G:C6     | 22:BA:251:A:C6     | 3.05                     | 0.45              |
| 22:BA:699:A:H4'    | 22:BA:1634:A:N7    | 2.30                     | 0.45              |
| 23:BB:15:A:O2'     | 23:BB:16:G:P       | 2.74                     | 0.45              |
| 24:BC:84:ASP:OD1   | 24:BC:84:ASP:C     | 2.55                     | 0.45              |
| 27:BF:148:ARG:CG   | 27:BF:149:VAL:H    | 2.29                     | 0.45              |
| 29:BH:72:ILE:HG23  | 29:BH:142:VAL:HG22 | 1.99                     | 0.45              |
| 29:BH:40:THR:O     | 29:BH:42:LYS:N     | 2.48                     | 0.45              |
| 30:BI:77:ALA:HB2   | 30:BI:132:THR:CG2  | 2.47                     | 0.45              |
| 31:BJ:98:GLU:OE2   | 31:BJ:126:ALA:HB2  | 2.16                     | 0.45              |
| 41:BT:91:GLN:HG3   | 41:BT:91:GLN:O     | 2.17                     | 0.45              |
| 1:CA:1091:U:H2'    | 1:CA:1093:A:OP2    | 2.16                     | 0.45              |
| 1:CA:1408:A:N1     | 1:CA:1494:G:C5     | 2.85                     | 0.45              |
| 1:CA:517:G:C8      | 1:CA:531:U:C4      | 3.04                     | 0.45              |
| 1:CA:505:G:OP2     | 1:CA:534:U:H2'     | 2.17                     | 0.45              |
| 1:CA:681:A:C2      | 1:CA:710:G:C4      | 3.05                     | 0.45              |
| 1:CA:706:A:O2'     | 11:CK:31:ILE:CD1   | 2.64                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:97:G:C6       | 1:CA:98:A:H1'      | 2.52                     | 0.45              |
| 2:CB:117:LEU:HB3   | 2:CB:141:LEU:HG    | 1.98                     | 0.45              |
| 2:CB:87:CYS:HB3    | 2:CB:222:ARG:HA    | 1.99                     | 0.45              |
| 6:CF:6:ILE:HD12    | 6:CF:6:ILE:N       | 2.31                     | 0.45              |
| 7:CG:126:ASP:N     | 7:CG:126:ASP:OD1   | 2.50                     | 0.45              |
| 18:CR:25:ASP:OD1   | 18:CR:25:ASP:N     | 2.50                     | 0.45              |
| 49:D1:9:ILE:CG2    | 49:D1:25:LYS:HB3   | 2.46                     | 0.45              |
| 22:DA:684:G:OP1    | 50:D2:16:HIS:ND1   | 2.49                     | 0.45              |
| 22:DA:1243:C:H2'   | 22:DA:1244:A:O4'   | 2.16                     | 0.45              |
| 22:DA:134:G:N2     | 22:DA:146:A:N3     | 2.64                     | 0.45              |
| 22:DA:1432:G:O2'   | 22:DA:1433:A:H5'   | 2.15                     | 0.45              |
| 22:DA:142:A:H2'    | 22:DA:143:C:C6     | 2.51                     | 0.45              |
| 22:DA:1801:A:C8    | 24:DC:262:ARG:NH2  | 2.85                     | 0.45              |
| 22:DA:1847:A:H2'   | 22:DA:1848:A:OP2   | 2.16                     | 0.45              |
| 22:DA:2141:G:N2    | 22:DA:2151:U:O2    | 2.50                     | 0.45              |
| 22:DA:2250:G:C8    | 22:DA:2250:G:O5'   | 2.70                     | 0.45              |
| 22:DA:2415:G:C6    | 22:DA:2416:C:N4    | 2.85                     | 0.45              |
| 22:DA:2574:G:N1    | 22:DA:2575:C:C2    | 2.85                     | 0.45              |
| 22:DA:2054:A:C2    | 22:DA:2616:C:C2    | 3.04                     | 0.45              |
| 22:DA:38:A:H4'     | 26:DE:45:ALA:HB2   | 1.97                     | 0.45              |
| 22:DA:445:C:H3'    | 22:DA:446:G:C8     | 2.52                     | 0.45              |
| 22:DA:49:A:N6      | 22:DA:177:G:C5     | 2.84                     | 0.45              |
| 22:DA:553:G:H2'    | 22:DA:554:U:O4'    | 2.17                     | 0.45              |
| 22:DA:693:A:H2'    | 22:DA:694:U:C6     | 2.50                     | 0.45              |
| 24:DC:158:ALA:HA   | 24:DC:195:VAL:HG22 | 1.99                     | 0.45              |
| 26:DE:146:VAL:HG12 | 26:DE:185:LYS:HB2  | 1.99                     | 0.45              |
| 26:DE:5:LEU:O      | 26:DE:6:LYS:C      | 2.55                     | 0.45              |
| 27:DF:29:PRO:HB2   | 27:DF:169:LEU:HD22 | 1.98                     | 0.45              |
| 27:DF:3:LYS:HD3    | 27:DF:101:GLU:OE2  | 2.17                     | 0.45              |
| 27:DF:44:ILE:HG21  | 27:DF:79:ILE:HG22  | 1.98                     | 0.45              |
| 30:DI:101:ILE:HG22 | 30:DI:102:SER:N    | 2.31                     | 0.45              |
| 30:DI:76:ALA:HA    | 30:DI:79:LEU:HB2   | 1.98                     | 0.45              |
| 36:DO:53:THR:HB    | 36:DO:65:THR:CG2   | 2.46                     | 0.45              |
| 36:DO:28:VAL:CG1   | 36:DO:94:ARG:HA    | 2.47                     | 0.45              |
| 40:DS:20:VAL:HG23  | 40:DS:39:THR:HG21  | 1.97                     | 0.45              |
| 40:DS:89:ALA:O     | 40:DS:90:LYS:HB2   | 2.16                     | 0.45              |
| 46:DY:28:LEU:CD2   | 46:DY:37:LEU:HD11  | 2.46                     | 0.45              |
| 22:DA:1184:U:OP1   | 47:DZ:30:ARG:NH2   | 2.50                     | 0.45              |
| 1:AA:1160:G:HO2'   | 1:AA:1161:C:P      | 2.39                     | 0.45              |
| 1:AA:1394:A:C5     | 1:AA:1501:C:H4'    | 2.52                     | 0.45              |
| 1:AA:438:U:C2      | 1:AA:494:G:C6      | 3.05                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AA:6:G:N3       | 1:AA:6:G:H3'      | 2.31                     | 0.45              |
| 1:AA:96:U:O2'     | 1:AA:97:G:P       | 2.75                     | 0.45              |
| 2:AB:151:ILE:CG2  | 2:AB:152:LYS:N    | 2.79                     | 0.45              |
| 2:AB:55:ALA:O     | 2:AB:59:LYS:N     | 2.44                     | 0.45              |
| 5:AE:80:THR:HB    | 5:AE:122:ASN:OD1  | 2.16                     | 0.45              |
| 6:AF:9:MET:CE     | 18:AR:65:LEU:HD22 | 2.47                     | 0.45              |
| 16:AP:4:ILE:HG13  | 16:AP:21:VAL:CG2  | 2.47                     | 0.45              |
| 17:AQ:50:ASN:O    | 17:AQ:51:ASN:C    | 2.53                     | 0.45              |
| 21:AU:41:PRO:O    | 21:AU:45:ARG:HD3  | 2.16                     | 0.45              |
| 53:B5:67:HIS:CD2  | 53:B5:188:ASP:HA  | 2.52                     | 0.45              |
| 22:BA:142:A:N7    | 22:BA:143:C:C4    | 2.85                     | 0.45              |
| 22:BA:152:A:H2'   | 22:BA:153:U:C6    | 2.52                     | 0.45              |
| 22:BA:223:A:C4    | 22:BA:422:A:C8    | 3.05                     | 0.45              |
| 22:BA:2315:G:H2'  | 22:BA:2316:G:C8   | 2.51                     | 0.45              |
| 22:BA:2419:U:OP1  | 51:B3:41:LYS:HE2  | 2.16                     | 0.45              |
| 22:BA:60:G:C8     | 22:BA:62:U:C6     | 3.04                     | 0.45              |
| 22:BA:626:A:H2'   | 33:BL:78:ARG:CZ   | 2.47                     | 0.45              |
| 22:BA:587:C:C6    | 22:BA:671:C:H1'   | 2.52                     | 0.45              |
| 22:BA:58:G:N2     | 22:BA:70:G:C4     | 2.85                     | 0.45              |
| 22:BA:909:A:O2'   | 22:BA:911:A:OP2   | 2.25                     | 0.45              |
| 22:BA:975:A:C4    | 22:BA:990:A:C5    | 3.05                     | 0.45              |
| 24:BC:220:VAL:HB  | 24:BC:225:MET:CE  | 2.47                     | 0.45              |
| 25:BD:101:PHE:C   | 25:BD:103:ASP:N   | 2.68                     | 0.45              |
| 26:BE:31:VAL:HG21 | 26:BE:104:ALA:CB  | 2.47                     | 0.45              |
| 26:BE:26:ALA:O    | 26:BE:27:LEU:C    | 2.54                     | 0.45              |
| 1:CA:1039:G:C6    | 1:CA:1040:U:N3    | 2.85                     | 0.45              |
| 1:CA:1070:U:C2    | 1:CA:1071:C:C5    | 3.04                     | 0.45              |
| 1:CA:1113:C:H4'   | 3:CC:14:ILE:HD12  | 1.99                     | 0.45              |
| 1:CA:1206:G:C6    | 1:CA:1207:G:C5    | 3.04                     | 0.45              |
| 1:CA:793:U:O2'    | 1:CA:1516:G:H1'   | 2.17                     | 0.45              |
| 1:CA:757:U:C2'    | 1:CA:758:C:O5'    | 2.65                     | 0.45              |
| 1:CA:764:C:C4     | 1:CA:765:G:C5     | 3.04                     | 0.45              |
| 1:CA:803:G:C5     | 1:CA:804:U:C4     | 3.05                     | 0.45              |
| 2:CB:16:PHE:N     | 2:CB:16:PHE:CD2   | 2.85                     | 0.45              |
| 3:CC:182:ILE:HD13 | 3:CC:203:PHE:HA   | 1.99                     | 0.45              |
| 5:CE:115:LEU:CD2  | 5:CE:123:VAL:HG21 | 2.47                     | 0.45              |
| 7:CG:145:ALA:O    | 7:CG:146:GLU:HB2  | 2.15                     | 0.45              |
| 7:CG:37:SER:OG    | 9:CI:43:THR:HG23  | 2.16                     | 0.45              |
| 12:CL:22:PRO:O    | 12:CL:24:LEU:N    | 2.45                     | 0.45              |
| 13:CM:33:ILE:HG22 | 13:CM:56:LEU:HD23 | 1.98                     | 0.45              |
| 16:CP:23:ASP:OD2  | 16:CP:25:ARG:HG2  | 2.17                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:DA:1016:G:C2    | 22:DA:1147:A:C2    | 3.04                     | 0.45              |
| 22:DA:1087:G:N1    | 22:DA:1089:A:C2    | 2.84                     | 0.45              |
| 22:DA:1140:C:C2'   | 22:DA:1141:U:H5'   | 2.47                     | 0.45              |
| 22:DA:1177:G:H2'   | 22:DA:1178:C:H4'   | 1.99                     | 0.45              |
| 22:DA:1286:A:N6    | 22:DA:1329:U:C2    | 2.85                     | 0.45              |
| 22:DA:1358:G:H2'   | 22:DA:1359:A:OP2   | 2.16                     | 0.45              |
| 22:DA:1818:U:H2'   | 24:DC:156:ARG:HD3  | 1.99                     | 0.45              |
| 22:DA:1998:A:H2'   | 22:DA:1999:C:O4'   | 2.16                     | 0.45              |
| 22:DA:2156:G:C6    | 22:DA:2157:G:N2    | 2.85                     | 0.45              |
| 22:DA:28:A:C2      | 22:DA:513:A:C8     | 3.05                     | 0.45              |
| 22:DA:30:G:C6      | 22:DA:31:C:N3      | 2.85                     | 0.45              |
| 22:DA:344:A:C2     | 22:DA:345:A:N7     | 2.85                     | 0.45              |
| 22:DA:663:G:O6     | 22:DA:664:G:C6     | 2.70                     | 0.45              |
| 23:DB:21:G:N2      | 23:DB:63:C:O2      | 2.50                     | 0.45              |
| 26:DE:148:ILE:HG21 | 26:DE:157:LEU:HD21 | 1.99                     | 0.45              |
| 29:DH:31:VAL:CG1   | 29:DH:32:PRO:HD3   | 2.47                     | 0.45              |
| 32:DK:39:ILE:HG13  | 32:DK:39:ILE:O     | 2.16                     | 0.45              |
| 32:DK:41:ILE:HD11  | 32:DK:86:LEU:HD22  | 1.98                     | 0.45              |
| 34:DM:124:LEU:HD23 | 34:DM:124:LEU:N    | 2.31                     | 0.45              |
| 39:DR:68:ARG:HD3   | 39:DR:92:TRP:CZ2   | 2.52                     | 0.45              |
| 41:DT:30:ILE:HD13  | 41:DT:32:LEU:CG    | 2.47                     | 0.45              |
| 1:AA:9:G:C2        | 1:AA:10:A:C8       | 3.05                     | 0.45              |
| 1:AA:1160:G:O6     | 1:AA:1181:G:C5     | 2.70                     | 0.45              |
| 1:AA:343:U:H2'     | 1:AA:345:C:C5      | 2.52                     | 0.45              |
| 1:AA:373:A:O2'     | 1:AA:374:A:H5'     | 2.15                     | 0.45              |
| 1:AA:624:C:C5      | 1:AA:625:U:C5      | 3.04                     | 0.45              |
| 1:AA:631:C:H5"     | 1:AA:632:U:H5'     | 1.98                     | 0.45              |
| 1:AA:659:U:N3      | 1:AA:660:C:C5      | 2.85                     | 0.45              |
| 1:AA:695:A:N1      | 1:AA:696:A:C2      | 2.85                     | 0.45              |
| 1:AA:908:A:C2      | 1:AA:909:A:C4      | 3.04                     | 0.45              |
| 1:AA:914:A:C5      | 1:AA:915:A:N7      | 2.84                     | 0.45              |
| 2:AB:148:LEU:C     | 2:AB:151:ILE:HG22  | 2.36                     | 0.45              |
| 2:AB:167:ASP:OD1   | 2:AB:168:HIS:N     | 2.50                     | 0.45              |
| 3:AC:19:ASN:OD1    | 3:AC:19:ASN:N      | 2.49                     | 0.45              |
| 3:AC:150:LYS:HG3   | 3:AC:201:TRP:CE3   | 2.52                     | 0.45              |
| 4:AD:160:GLU:O     | 4:AD:162:ALA:N     | 2.49                     | 0.45              |
| 4:AD:105:MET:CG    | 4:AD:171:LEU:HD22  | 2.47                     | 0.45              |
| 5:AE:153:VAL:O     | 5:AE:156:LYS:HB2   | 2.17                     | 0.45              |
| 8:AH:88:ARG:O      | 8:AH:92:LEU:HG     | 2.17                     | 0.45              |
| 13:AM:80:LEU:CD2   | 13:AM:87:ARG:HB2   | 2.46                     | 0.45              |
| 14:AN:64:CYS:SG    | 14:AN:80:SER:HB3   | 2.57                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 17:AQ:16:LYS:CA   | 17:AQ:17:MET:SD   | 3.05                     | 0.45              |
| 22:BA:1109:C:C5   | 22:BA:1110:G:C6   | 3.05                     | 0.45              |
| 22:BA:1434:A:C2   | 22:BA:1435:G:C5   | 3.04                     | 0.45              |
| 22:BA:1324:G:H1'  | 22:BA:1616:A:N6   | 2.32                     | 0.45              |
| 22:BA:1851:U:O2'  | 22:BA:1852:U:H5'  | 2.17                     | 0.45              |
| 22:BA:1857:G:N3   | 22:BA:1884:G:C2   | 2.85                     | 0.45              |
| 22:BA:1921:G:N2   | 22:BA:1922:G:C8   | 2.84                     | 0.45              |
| 22:BA:2177:C:N4   | 22:BA:2178:C:O2   | 2.50                     | 0.45              |
| 22:BA:2192:U:C5   | 22:BA:2193:G:C8   | 3.05                     | 0.45              |
| 22:BA:2311:A:C2   | 27:BF:41:GLY:CA   | 3.00                     | 0.45              |
| 22:BA:559:G:H2'   | 22:BA:560:C:O4'   | 2.17                     | 0.45              |
| 22:BA:7:G:C6      | 22:BA:8:C:C4      | 3.05                     | 0.45              |
| 22:BA:858:G:C4    | 22:BA:2268:A:C2   | 3.05                     | 0.45              |
| 22:BA:997:G:OP1   | 38:BQ:92:ARG:HG3  | 2.15                     | 0.45              |
| 23:BB:78:A:C2     | 23:BB:99:A:C4     | 3.05                     | 0.45              |
| 24:BC:28:LYS:HD3  | 24:BC:28:LYS:N    | 2.32                     | 0.45              |
| 28:BG:94:TYR:HA   | 28:BG:106:SER:O   | 2.16                     | 0.45              |
| 29:BH:14:SER:OG   | 29:BH:17:ASP:OD1  | 2.29                     | 0.45              |
| 30:BI:44:ALA:O    | 30:BI:45:LYS:HG3  | 2.17                     | 0.45              |
| 32:BK:23:LYS:HB3  | 32:BK:40:LYS:HB3  | 1.98                     | 0.45              |
| 39:BR:66:HIS:ND1  | 39:BR:94:THR:CG2  | 2.80                     | 0.45              |
| 34:BM:20:LEU:HD12 | 43:BV:81:PRO:CG   | 2.46                     | 0.45              |
| 1:CA:1258:G:H2'   | 1:CA:1259:C:C6    | 2.51                     | 0.45              |
| 1:CA:920:U:C2     | 1:CA:921:U:C5     | 3.05                     | 0.45              |
| 1:CA:9:G:OP2      | 5:CE:126:LYS:CE   | 2.65                     | 0.45              |
| 5:CE:101:GLU:HA   | 5:CE:122:ASN:CB   | 2.46                     | 0.45              |
| 5:CE:16:ILE:HD12  | 5:CE:16:ILE:N     | 2.32                     | 0.45              |
| 6:CF:37:HIS:O     | 6:CF:38:ARG:HB3   | 2.17                     | 0.45              |
| 1:CA:1291:U:OP1   | 7:CG:37:SER:CB    | 2.65                     | 0.45              |
| 9:CI:49:ARG:C     | 9:CI:49:ARG:HD3   | 2.37                     | 0.45              |
| 9:CI:88:MET:O     | 9:CI:88:MET:CG    | 2.65                     | 0.45              |
| 11:CK:82:LEU:O    | 11:CK:82:LEU:HD23 | 2.17                     | 0.45              |
| 14:CN:51:LEU:O    | 14:CN:53:ARG:N    | 2.50                     | 0.45              |
| 19:CS:51:VAL:O    | 19:CS:58:VAL:HG13 | 2.17                     | 0.45              |
| 22:DA:136:G:N2    | 22:DA:144:A:C5    | 2.85                     | 0.45              |
| 22:DA:1623:G:C6   | 22:DA:1624:U:C4   | 3.05                     | 0.45              |
| 22:DA:186:G:C2    | 22:DA:211:C:O2    | 2.70                     | 0.45              |
| 22:DA:192:C:H2'   | 22:DA:193:U:H5'   | 1.99                     | 0.45              |
| 22:DA:2284:A:O2'  | 22:DA:2288:A:N1   | 2.37                     | 0.45              |
| 22:DA:2751:G:H2'  | 22:DA:2751:G:N3   | 2.32                     | 0.45              |
| 22:DA:515:A:H2'   | 22:DA:516:C:H5'   | 1.98                     | 0.45              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:DA:533:G:C5    | 22:DA:534:U:C4    | 3.04                     | 0.45              |
| 22:DA:82:U:O2     | 22:DA:83:A:C8     | 2.69                     | 0.45              |
| 29:DH:93:SER:HB3  | 29:DH:123:ARG:HG3 | 1.99                     | 0.45              |
| 29:DH:86:ASP:C    | 29:DH:88:GLY:H    | 2.19                     | 0.45              |
| 30:DI:57:VAL:HG23 | 30:DI:71:THR:CA   | 2.47                     | 0.45              |
| 1:AA:1118:U:C1'   | 1:AA:1179:A:C4    | 3.00                     | 0.45              |
| 1:AA:126:G:O2'    | 1:AA:635:A:H4'    | 2.17                     | 0.45              |
| 1:AA:221:C:C2     | 1:AA:222:C:C5     | 3.05                     | 0.45              |
| 1:AA:224:U:H2'    | 1:AA:225:C:C6     | 2.51                     | 0.45              |
| 1:AA:457:G:C6     | 1:AA:458:U:C4     | 3.05                     | 0.45              |
| 1:AA:691:G:O6     | 11:AK:57:LYS:NZ   | 2.50                     | 0.45              |
| 1:AA:765:G:C6     | 1:AA:812:G:C4     | 3.05                     | 0.45              |
| 3:AC:39:VAL:O     | 3:AC:43:LEU:HB2   | 2.16                     | 0.45              |
| 3:AC:42:TYR:CZ    | 3:AC:90:VAL:HG21  | 2.52                     | 0.45              |
| 4:AD:58:LYS:HE2   | 4:AD:69:GLU:OE2   | 2.17                     | 0.45              |
| 5:AE:13:GLU:HB2   | 5:AE:39:VAL:HG12  | 1.99                     | 0.45              |
| 10:AJ:57:VAL:CG2  | 10:AJ:58:ASN:N    | 2.79                     | 0.45              |
| 10:AJ:65:TYR:OH   | 14:AN:85:ARG:HD2  | 2.17                     | 0.45              |
| 22:BA:1171:G:C5   | 22:BA:1172:C:C4   | 3.05                     | 0.45              |
| 22:BA:1169:A:N1   | 22:BA:1180:U:O4   | 2.50                     | 0.45              |
| 22:BA:1242:U:H2'  | 22:BA:1243:C:C6   | 2.52                     | 0.45              |
| 22:BA:1795:C:C4   | 22:BA:1796:U:C5   | 3.05                     | 0.45              |
| 22:BA:2094:A:C2   | 22:BA:2196:C:C2   | 3.05                     | 0.45              |
| 22:BA:2258:C:H4'  | 22:BA:2259:U:OP2  | 2.17                     | 0.45              |
| 22:BA:2694:G:C5   | 22:BA:2695:U:C4   | 3.05                     | 0.45              |
| 22:BA:2804:U:H2'  | 22:BA:2805:C:C6   | 2.52                     | 0.45              |
| 22:BA:2888:C:O2   | 22:BA:2888:C:C2'  | 2.64                     | 0.45              |
| 22:BA:441:U:H2'   | 22:BA:442:G:C8    | 2.52                     | 0.45              |
| 22:BA:55:G:N2     | 22:BA:56:A:C4     | 2.85                     | 0.45              |
| 24:BC:264:ASP:O   | 24:BC:265:LYS:C   | 2.55                     | 0.45              |
| 29:BH:76:GLU:HA   | 29:BH:142:VAL:CG1 | 2.46                     | 0.45              |
| 35:BN:72:ASP:O    | 35:BN:76:VAL:HG12 | 2.17                     | 0.45              |
| 38:BQ:49:ASP:OD2  | 38:BQ:52:GLN:OE1  | 2.35                     | 0.45              |
| 45:BX:78:TYR:CD1  | 45:BX:78:TYR:OXT  | 2.70                     | 0.45              |
| 1:CA:1027:C:N4    | 1:CA:1034:G:O6    | 2.50                     | 0.45              |
| 1:CA:16:A:C2      | 1:CA:17:U:C6      | 3.05                     | 0.45              |
| 1:CA:218:U:C2'    | 1:CA:219:U:H5'    | 2.47                     | 0.45              |
| 1:CA:240:G:OP1    | 1:CA:240:G:H4'    | 2.16                     | 0.45              |
| 1:CA:421:U:H4'    | 1:CA:421:U:OP1    | 2.17                     | 0.45              |
| 1:CA:444:G:C6     | 1:CA:445:G:N7     | 2.85                     | 0.45              |
| 1:CA:541:G:H2'    | 1:CA:542:G:O4'    | 2.17                     | 0.45              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:778:G:C6      | 1:CA:779:C:N3      | 2.85                     | 0.45              |
| 1:CA:782:A:C8      | 1:CA:783:C:C5      | 3.05                     | 0.45              |
| 1:CA:745:G:H5''    | 1:CA:851:G:O2'     | 2.17                     | 0.45              |
| 2:CB:10:LEU:HD23   | 2:CB:12:ALA:O      | 2.17                     | 0.45              |
| 2:CB:71:GLY:HA3    | 2:CB:164:ILE:HG21  | 1.99                     | 0.45              |
| 4:CD:35:GLU:O      | 4:CD:37:ALA:N      | 2.45                     | 0.45              |
| 6:CF:17:GLN:O      | 6:CF:21:MET:HG3    | 2.17                     | 0.45              |
| 22:DA:1062:G:C2    | 22:DA:1063:G:N1    | 2.85                     | 0.45              |
| 22:DA:1194:A:C2'   | 22:DA:1195:G:O5'   | 2.64                     | 0.45              |
| 22:DA:1448:G:C4    | 22:DA:1449:G:C8    | 3.05                     | 0.45              |
| 22:DA:1526:C:N4    | 22:DA:1527:G:C6    | 2.85                     | 0.45              |
| 22:DA:1598:A:H2'   | 22:DA:1599:U:C6    | 2.52                     | 0.45              |
| 22:DA:185:G:C6     | 22:DA:212:G:N2     | 2.85                     | 0.45              |
| 22:DA:1965:C:H3'   | 22:DA:1966:A:C8    | 2.51                     | 0.45              |
| 22:DA:1265:A:N6    | 22:DA:2014:A:OP2   | 2.40                     | 0.45              |
| 22:DA:2059:A:H4'   | 26:DE:64:GLY:O     | 2.16                     | 0.45              |
| 22:DA:2195:U:C2    | 22:DA:2196:C:C6    | 3.04                     | 0.45              |
| 22:DA:2345:G:C5    | 22:DA:2381:A:C2    | 3.05                     | 0.45              |
| 22:DA:2729:G:H2'   | 22:DA:2730:C:O4'   | 2.16                     | 0.45              |
| 22:DA:351:C:H2'    | 22:DA:352:A:C8     | 2.52                     | 0.45              |
| 22:DA:810:U:O4     | 33:DL:30:THR:HG22  | 2.17                     | 0.45              |
| 23:DB:66:A:N6      | 23:DB:107:G:H2'    | 2.32                     | 0.45              |
| 57:DA:3238:HOH:O   | 26:DE:47:LYS:HD2   | 2.17                     | 0.45              |
| 28:DG:121:ILE:HD12 | 28:DG:141:ILE:HG22 | 1.99                     | 0.45              |
| 29:DH:83:LYS:HG3   | 29:DH:149:GLU:HG3  | 1.94                     | 0.45              |
| 30:DI:24:VAL:HB    | 30:DI:28:LEU:HD23  | 1.99                     | 0.45              |
| 31:DJ:59:ALA:O     | 31:DJ:62:VAL:HG12  | 2.16                     | 0.45              |
| 33:DL:119:PRO:HB3  | 33:DL:139:GLY:HA3  | 1.98                     | 0.45              |
| 35:DN:36:THR:OG1   | 35:DN:37:THR:N     | 2.49                     | 0.45              |
| 37:DP:39:ARG:HG3   | 37:DP:40:LEU:H     | 1.80                     | 0.45              |
| 41:DT:69:ARG:HA    | 41:DT:74:ILE:HG22  | 1.99                     | 0.45              |
| 41:DT:73:ARG:HA    | 41:DT:73:ARG:NH2   | 2.32                     | 0.45              |
| 1:AA:114:U:H2'     | 1:AA:115:G:C8      | 2.52                     | 0.45              |
| 1:AA:1243:C:H2'    | 1:AA:1244:G:C8     | 2.52                     | 0.45              |
| 1:AA:203:G:C2      | 1:AA:215:C:C2      | 3.05                     | 0.45              |
| 1:AA:716:A:C6      | 1:AA:717:U:N3      | 2.85                     | 0.45              |
| 2:AB:72:THR:O      | 2:AB:73:LYS:HB3    | 2.16                     | 0.45              |
| 4:AD:147:GLU:O     | 4:AD:150:LYS:N     | 2.50                     | 0.45              |
| 4:AD:160:GLU:C     | 4:AD:162:ALA:H     | 2.20                     | 0.45              |
| 8:AH:34:VAL:O      | 8:AH:36:ILE:N      | 2.49                     | 0.45              |
| 9:AI:114:LYS:NZ    | 9:AI:118:LEU:O     | 2.44                     | 0.45              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 9:AI:30:ILE:HD11   | 9:AI:38:TYR:CB      | 2.47                     | 0.45              |
| 10:AJ:52:LEU:HB2   | 14:AN:81:ARG:HD2    | 1.99                     | 0.45              |
| 13:AM:12:HIS:HA    | 13:AM:44:LYS:HE3    | 1.99                     | 0.45              |
| 1:AA:310:G:H5''    | 16:AP:31:ARG:HB2    | 1.97                     | 0.45              |
| 17:AQ:12:VAL:CG1   | 17:AQ:13:VAL:N      | 2.80                     | 0.45              |
| 20:AT:44:LYS:NZ    | 20:AT:86:LEU:O      | 2.43                     | 0.45              |
| 53:B5:64:SER:O     | 53:B5:65:LEU:HB3    | 2.17                     | 0.45              |
| 22:BA:1922:G:N3    | 22:BA:1922:G:C2'    | 2.80                     | 0.45              |
| 22:BA:1972:G:C2    | 22:BA:1973:G:C5     | 3.05                     | 0.45              |
| 22:BA:187:G:C2     | 22:BA:210:C:C2      | 3.05                     | 0.45              |
| 22:BA:2061:G:O6    | 55:BA:3001:DOL:H132 | 2.16                     | 0.45              |
| 22:BA:982:C:H5''   | 22:BA:983:A:P       | 2.57                     | 0.45              |
| 28:BG:99:LYS:O     | 28:BG:100:GLY:C     | 2.55                     | 0.45              |
| 29:BH:12:LEU:HG    | 29:BH:13:GLY:N      | 2.31                     | 0.45              |
| 30:BI:116:ASP:OD2  | 30:BI:117:MET:N     | 2.50                     | 0.45              |
| 32:BK:107:LEU:C    | 32:BK:109:SER:N     | 2.70                     | 0.45              |
| 34:BM:132:THR:HG22 | 34:BM:133:LYS:N     | 2.31                     | 0.45              |
| 38:BQ:41:LYS:HA    | 38:BQ:44:GLN:OE1    | 2.16                     | 0.45              |
| 46:BY:56:LEU:O     | 46:BY:57:LEU:C      | 2.54                     | 0.45              |
| 1:CA:1166:G:N1     | 1:CA:1169:A:OP2     | 2.45                     | 0.45              |
| 1:CA:33:A:C4       | 1:CA:34:C:C5        | 3.04                     | 0.45              |
| 1:CA:355:C:H2'     | 1:CA:356:A:O4'      | 2.17                     | 0.45              |
| 1:CA:714:G:H2'     | 1:CA:715:A:C8       | 2.52                     | 0.45              |
| 5:CE:101:GLU:HA    | 5:CE:122:ASN:HB3    | 1.99                     | 0.45              |
| 5:CE:131:THR:O     | 5:CE:132:ASN:C      | 2.54                     | 0.45              |
| 12:CL:86:ARG:NH1   | 12:CL:88:LYS:HA     | 2.32                     | 0.45              |
| 13:CM:96:PRO:HB2   | 13:CM:100:GLN:OE1   | 2.16                     | 0.45              |
| 19:CS:40:ILE:HD13  | 19:CS:66:MET:HB3    | 1.97                     | 0.45              |
| 21:CU:34:ARG:CD    | 21:CU:35:ARG:HB2    | 2.47                     | 0.45              |
| 22:DA:1095:A:C2    | 22:DA:1096:A:C2     | 3.05                     | 0.45              |
| 22:DA:1345:C:H5'   | 22:DA:1396:U:C5     | 2.52                     | 0.45              |
| 22:DA:1509:A:O2'   | 22:DA:1510:G:O5'    | 2.34                     | 0.45              |
| 22:DA:1477:A:N6    | 22:DA:1514:G:H1'    | 2.30                     | 0.45              |
| 22:DA:1559:U:H4'   | 22:DA:1560:G:OP2    | 2.17                     | 0.45              |
| 22:DA:1567:G:H2'   | 24:DC:85:PRO:HG3    | 1.99                     | 0.45              |
| 22:DA:1731:G:C6    | 22:DA:1733:G:N7     | 2.85                     | 0.45              |
| 22:DA:1767:G:N1    | 22:DA:1986:C:C4     | 2.85                     | 0.45              |
| 22:DA:207:A:C4     | 22:DA:208:C:C6      | 3.05                     | 0.45              |
| 22:DA:2252:G:H2'   | 22:DA:2253:G:O4'    | 2.16                     | 0.45              |
| 22:DA:2425:A:H4'   | 22:DA:2426:A:O5'    | 2.17                     | 0.45              |
| 22:DA:2513:A:C4    | 22:DA:2514:U:C5     | 3.05                     | 0.45              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:DA:372:G:N2    | 22:DA:401:A:OP2    | 2.43                     | 0.45              |
| 22:DA:416:U:H2'   | 22:DA:417:C:O4'    | 2.17                     | 0.45              |
| 22:DA:469:G:O6    | 50:D2:37:LYS:NZ    | 2.48                     | 0.45              |
| 22:DA:84:A:N6     | 22:DA:99:U:H4'     | 2.32                     | 0.45              |
| 22:DA:1830:C:H5'  | 24:DC:15:HIS:CD2   | 2.52                     | 0.45              |
| 25:DD:125:TRP:O   | 25:DD:126:ASN:HB2  | 2.17                     | 0.45              |
| 29:DH:15:LEU:HD22 | 29:DH:15:LEU:N     | 2.32                     | 0.45              |
| 37:DP:106:LYS:HA  | 37:DP:109:ARG:HD2  | 1.98                     | 0.45              |
| 41:DT:62:VAL:HG12 | 41:DT:63:VAL:N     | 2.32                     | 0.45              |
| 42:DU:7:ARG:HG3   | 42:DU:8:ASP:H      | 1.82                     | 0.45              |
| 22:DA:1364:G:OP1  | 45:DX:3:ARG:CG     | 2.65                     | 0.45              |
| 1:AA:992:U:O2     | 1:AA:1043:G:N7     | 2.50                     | 0.44              |
| 1:AA:1410:A:H2'   | 1:AA:1411:C:C6     | 2.52                     | 0.44              |
| 1:AA:202:G:O2'    | 1:AA:468:A:H2'     | 2.17                     | 0.44              |
| 1:AA:631:C:H5''   | 1:AA:632:U:C5'     | 2.46                     | 0.44              |
| 1:AA:854:U:C6     | 1:AA:871:U:O4      | 2.69                     | 0.44              |
| 1:AA:858:G:C6     | 1:AA:869:G:C8      | 3.05                     | 0.44              |
| 2:AB:84:ALA:O     | 2:AB:89:GLN:CB     | 2.65                     | 0.44              |
| 3:AC:84:VAL:CG1   | 3:AC:101:ILE:HG21  | 2.47                     | 0.44              |
| 4:AD:50:ASP:C     | 4:AD:50:ASP:OD2    | 2.55                     | 0.44              |
| 6:AF:45:ARG:O     | 6:AF:56:LYS:HA     | 2.17                     | 0.44              |
| 8:AH:10:MET:HE2   | 8:AH:33:LYS:HD3    | 1.99                     | 0.44              |
| 8:AH:95:VAL:CG1   | 8:AH:96:MET:N      | 2.80                     | 0.44              |
| 12:AL:50:ARG:HG3  | 12:AL:90:LEU:HD11  | 1.99                     | 0.44              |
| 13:AM:114:LYS:CB  | 13:AM:115:PRO:CD   | 2.94                     | 0.44              |
| 17:AQ:12:VAL:O    | 17:AQ:13:VAL:CG1   | 2.63                     | 0.44              |
| 1:AA:196:A:OP1    | 20:AT:64:LYS:CE    | 2.66                     | 0.44              |
| 21:AU:11:PRO:C    | 21:AU:12:PHE:CD2   | 2.90                     | 0.44              |
| 22:BA:1022:G:C5   | 22:BA:1140:C:C4    | 3.05                     | 0.44              |
| 22:BA:1360:G:O6   | 22:BA:1372:U:C2    | 2.70                     | 0.44              |
| 22:BA:1386:C:H5'' | 22:BA:1396:U:O2    | 2.17                     | 0.44              |
| 22:BA:2714:G:C5   | 22:BA:2715:C:C5    | 3.05                     | 0.44              |
| 22:BA:271:G:C4'   | 22:BA:272:A:OP1    | 2.65                     | 0.44              |
| 22:BA:532:A:H2'   | 22:BA:532:A:N3     | 2.32                     | 0.44              |
| 22:BA:55:G:C2     | 22:BA:56:A:C5      | 3.06                     | 0.44              |
| 22:BA:747:U:N3    | 22:BA:2613:U:C4    | 2.85                     | 0.44              |
| 28:BG:118:PRO:O   | 28:BG:119:ALA:C    | 2.55                     | 0.44              |
| 30:BI:116:ASP:O   | 30:BI:117:MET:HG2  | 2.17                     | 0.44              |
| 30:BI:117:MET:CE  | 30:BI:129:ILE:HD11 | 2.48                     | 0.44              |
| 30:BI:19:ASN:ND2  | 30:BI:35:ILE:O     | 2.51                     | 0.44              |
| 37:BP:113:ARG:O   | 37:BP:114:LEU:O    | 2.35                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CA:1287:A:C6    | 1:CA:1288:A:C6    | 3.05                     | 0.44              |
| 1:CA:1411:C:H2'   | 1:CA:1412:C:H6    | 1.81                     | 0.44              |
| 1:CA:197:A:C6     | 1:CA:221:C:H4'    | 2.52                     | 0.44              |
| 1:CA:951:G:C6     | 1:CA:952:U:C4     | 3.05                     | 0.44              |
| 2:CB:118:GLU:HA   | 2:CB:121:SER:OG   | 2.17                     | 0.44              |
| 4:CD:5:LEU:CD1    | 4:CD:5:LEU:N      | 2.80                     | 0.44              |
| 6:CF:37:HIS:CD2   | 6:CF:65:GLU:HB2   | 2.52                     | 0.44              |
| 8:CH:59:LEU:HD12  | 8:CH:60:GLU:N     | 2.32                     | 0.44              |
| 11:CK:19:GLY:O    | 11:CK:82:LEU:HA   | 2.17                     | 0.44              |
| 12:CL:72:HIS:ND1  | 12:CL:74:LEU:HB2  | 2.32                     | 0.44              |
| 1:CA:1226:C:N4    | 13:CM:103:LYS:HB2 | 2.33                     | 0.44              |
| 14:CN:51:LEU:HB3  | 14:CN:52:PRO:HD2  | 1.99                     | 0.44              |
| 15:CO:35:GLN:NE2  | 15:CO:39:LEU:HD21 | 2.32                     | 0.44              |
| 20:CT:3:ASN:O     | 20:CT:4:ILE:C     | 2.55                     | 0.44              |
| 51:D3:32:ILE:HG22 | 51:D3:35:LYS:HD2  | 1.99                     | 0.44              |
| 22:DA:1246:A:O2'  | 26:DE:40:ARG:NH2  | 2.51                     | 0.44              |
| 22:DA:1401:G:C5   | 22:DA:1402:U:C5   | 3.05                     | 0.44              |
| 22:DA:1480:C:C4   | 22:DA:1481:U:C4   | 3.05                     | 0.44              |
| 22:DA:1444:G:N2   | 22:DA:1548:A:N3   | 2.65                     | 0.44              |
| 22:DA:1428:C:C4   | 22:DA:1569:A:H5'' | 2.52                     | 0.44              |
| 22:DA:1773:A:C2   | 22:DA:1978:A:C2   | 3.05                     | 0.44              |
| 22:DA:188:G:C2    | 22:DA:209:C:N3    | 2.85                     | 0.44              |
| 22:DA:1827:U:C4'  | 22:DA:1970:A:HO2' | 2.29                     | 0.44              |
| 22:DA:2112:G:H5'  | 22:DA:2113:U:OP2  | 2.17                     | 0.44              |
| 22:DA:2307:G:N2   | 22:DA:2312:U:C4   | 2.85                     | 0.44              |
| 22:DA:2683:C:H4'  | 25:DD:13:ARG:NH1  | 2.31                     | 0.44              |
| 22:DA:306:U:O4    | 22:DA:307:G:C6    | 2.70                     | 0.44              |
| 22:DA:546:U:O2    | 22:DA:546:U:H2'   | 2.17                     | 0.44              |
| 22:DA:682:G:N3    | 22:DA:682:G:H2'   | 2.31                     | 0.44              |
| 22:DA:81:G:N7     | 22:DA:82:U:C4     | 2.85                     | 0.44              |
| 22:DA:868:U:C4    | 22:DA:869:G:N7    | 2.85                     | 0.44              |
| 25:DD:151:THR:HB  | 25:DD:152:PRO:HD2 | 1.98                     | 0.44              |
| 29:DH:5:LEU:CD1   | 29:DH:13:GLY:CA   | 2.95                     | 0.44              |
| 32:DK:32:TYR:CD2  | 32:DK:32:TYR:N    | 2.85                     | 0.44              |
| 34:DM:67:VAL:HG11 | 34:DM:96:ILE:HD12 | 1.99                     | 0.44              |
| 35:DN:84:GLY:N    | 35:DN:85:PRO:HD2  | 2.32                     | 0.44              |
| 37:DP:30:VAL:HG12 | 37:DP:31:TRP:O    | 2.18                     | 0.44              |
| 40:DS:22:ASP:OD2  | 40:DS:22:ASP:N    | 2.50                     | 0.44              |
| 57:DB:307:HOH:O   | 43:DV:14:LYS:HD2  | 2.17                     | 0.44              |
| 1:AA:102:G:C4     | 1:AA:103:U:C5     | 3.06                     | 0.44              |
| 1:AA:1081:A:P     | 5:AE:21:VAL:HG21  | 2.57                     | 0.44              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:AA:1130:A:H1'    | 1:AA:1146:A:C2    | 2.53                     | 0.44              |
| 1:AA:1263:C:H2'    | 1:AA:1264:U:C6    | 2.52                     | 0.44              |
| 1:AA:1309:G:C6     | 1:AA:1310:G:C5    | 3.05                     | 0.44              |
| 1:AA:1322:C:O4'    | 1:AA:1322:C:O2    | 2.35                     | 0.44              |
| 1:AA:1353:G:C2     | 1:AA:1354:U:C6    | 3.05                     | 0.44              |
| 1:AA:412:A:H4'     | 1:AA:413:G:OP1    | 2.17                     | 0.44              |
| 1:AA:423:G:H2'     | 1:AA:424:G:O4'    | 2.17                     | 0.44              |
| 1:AA:472:U:C4      | 1:AA:473:U:O4     | 2.70                     | 0.44              |
| 1:AA:549:C:C2      | 1:AA:550:G:C8     | 3.05                     | 0.44              |
| 1:AA:587:G:C2      | 1:AA:755:G:C6     | 3.05                     | 0.44              |
| 1:AA:587:G:N2      | 1:AA:755:G:C4     | 2.85                     | 0.44              |
| 1:AA:598:U:H4'     | 8:AH:86:TYR:CG    | 2.52                     | 0.44              |
| 1:AA:800:G:C6      | 57:AA:1814:HOH:O  | 2.54                     | 0.44              |
| 3:AC:26:THR:O      | 3:AC:27:LYS:C     | 2.53                     | 0.44              |
| 3:AC:60:PRO:O      | 3:AC:61:ALA:O     | 2.35                     | 0.44              |
| 3:AC:85:GLU:HA     | 3:AC:88:ARG:CZ    | 2.48                     | 0.44              |
| 5:AE:115:LEU:CD2   | 5:AE:123:VAL:HG21 | 2.47                     | 0.44              |
| 5:AE:20:ARG:HG3    | 5:AE:21:VAL:N     | 2.32                     | 0.44              |
| 5:AE:84:PRO:HA     | 5:AE:98:PRO:HD3   | 1.99                     | 0.44              |
| 10:AJ:36:VAL:HA    | 10:AJ:75:ASP:O    | 2.17                     | 0.44              |
| 11:AK:56:ARG:O     | 11:AK:59:THR:HG23 | 2.17                     | 0.44              |
| 11:AK:72:ASP:O     | 11:AK:73:ALA:HB2  | 2.18                     | 0.44              |
| 12:AL:59:ASN:C     | 12:AL:59:ASN:OD1  | 2.54                     | 0.44              |
| 1:AA:1329:A:H5''   | 13:AM:26:GLY:N    | 2.33                     | 0.44              |
| 19:AS:3:ARG:O      | 19:AS:4:SER:CB    | 2.65                     | 0.44              |
| 53:B5:65:LEU:HD21  | 53:B5:195:ARG:CB  | 2.48                     | 0.44              |
| 22:BA:1092:C:N4    | 22:BA:1098:A:H62  | 2.14                     | 0.44              |
| 22:BA:1350:C:C2    | 22:BA:1382:G:C2   | 3.06                     | 0.44              |
| 22:BA:1378:A:N3    | 22:BA:1380:G:C8   | 2.86                     | 0.44              |
| 22:BA:2172:U:OP2   | 22:BA:2173:A:H8   | 2.00                     | 0.44              |
| 22:BA:2267:A:H5''  | 22:BA:2268:A:H5'  | 1.99                     | 0.44              |
| 22:BA:2720:U:C2    | 22:BA:2872:A:C6   | 3.05                     | 0.44              |
| 22:BA:468:G:O6     | 22:BA:469:G:C2    | 2.71                     | 0.44              |
| 22:BA:864:G:O2'    | 22:BA:865:C:H5'   | 2.16                     | 0.44              |
| 24:BC:141:VAL:HG11 | 24:BC:190:ALA:CB  | 2.47                     | 0.44              |
| 25:BD:13:ARG:HD2   | 25:BD:15:PHE:CE1  | 2.51                     | 0.44              |
| 25:BD:177:VAL:HG23 | 25:BD:177:VAL:O   | 2.18                     | 0.44              |
| 26:BE:48:THR:HG22  | 26:BE:86:ALA:HB3  | 1.99                     | 0.44              |
| 27:BF:17:MET:CE    | 27:BF:22:TYR:HB2  | 2.47                     | 0.44              |
| 28:BG:2:SER:C      | 28:BG:4:VAL:N     | 2.66                     | 0.44              |
| 29:BH:57:LYS:CG    | 29:BH:58:LEU:N    | 2.81                     | 0.44              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 35:BN:31:HIS:O     | 35:BN:33:ILE:N    | 2.50                     | 0.44              |
| 36:BO:59:ALA:O     | 36:BO:60:GLU:C    | 2.55                     | 0.44              |
| 31:BJ:42:ALA:O     | 38:BQ:64:ARG:HG2  | 2.17                     | 0.44              |
| 1:CA:178:C:H2'     | 1:CA:179:A:O4'    | 2.17                     | 0.44              |
| 1:CA:251:G:N1      | 1:CA:266:G:C6     | 2.85                     | 0.44              |
| 1:CA:517:G:H5'     | 1:CA:519:C:C2     | 2.51                     | 0.44              |
| 1:CA:540:G:C6      | 1:CA:541:G:C5     | 3.05                     | 0.44              |
| 1:CA:632:U:H2'     | 1:CA:633:G:OP1    | 2.17                     | 0.44              |
| 1:CA:937:A:C2      | 1:CA:1379:G:O6    | 2.69                     | 0.44              |
| 2:CB:148:LEU:N     | 2:CB:148:LEU:HD12 | 2.33                     | 0.44              |
| 3:CC:117:ALA:HB1   | 3:CC:187:SER:HB2  | 1.98                     | 0.44              |
| 4:CD:155:VAL:HA    | 4:CD:158:ALA:HB3  | 2.00                     | 0.44              |
| 5:CE:104:GLY:O     | 5:CE:105:ILE:HG23 | 2.17                     | 0.44              |
| 5:CE:155:ALA:C     | 5:CE:156:LYS:HG3  | 2.36                     | 0.44              |
| 9:CI:30:ILE:HD13   | 9:CI:39:PHE:CE2   | 2.52                     | 0.44              |
| 9:CI:46:MET:O      | 9:CI:49:ARG:HB3   | 2.17                     | 0.44              |
| 11:CK:43:GLY:HA3   | 11:CK:74:VAL:HG12 | 1.99                     | 0.44              |
| 11:CK:25:ALA:O     | 11:CK:89:PRO:O    | 2.36                     | 0.44              |
| 14:CN:41:ARG:HG2   | 14:CN:42:TRP:N    | 2.31                     | 0.44              |
| 19:CS:36:ARG:NH1   | 19:CS:72:GLY:HA3  | 2.32                     | 0.44              |
| 48:D0:48:TYR:CE2   | 48:D0:53:LYS:HD3  | 2.52                     | 0.44              |
| 50:D2:30:VAL:O     | 50:D2:34:ARG:HG3  | 2.17                     | 0.44              |
| 22:DA:1569:A:C6    | 22:DA:1570:A:C2   | 3.05                     | 0.44              |
| 22:DA:2103:C:H2'   | 22:DA:2104:C:C5   | 2.53                     | 0.44              |
| 22:DA:2211:A:C4'   | 22:DA:2212:A:OP1  | 2.65                     | 0.44              |
| 22:DA:2297:A:N7    | 22:DA:2320:U:C4   | 2.85                     | 0.44              |
| 22:DA:235:U:C4     | 22:DA:430:A:C2    | 3.05                     | 0.44              |
| 22:DA:2412:A:H5''  | 22:DA:2413:G:OP2  | 2.17                     | 0.44              |
| 22:DA:2478:A:C8    | 22:DA:2529:G:N7   | 2.85                     | 0.44              |
| 22:DA:613:A:OP2    | 22:DA:614:A:N7    | 2.51                     | 0.44              |
| 22:DA:465:G:N2     | 22:DA:684:G:H1'   | 2.32                     | 0.44              |
| 22:DA:728:G:C2     | 22:DA:730:A:C4    | 3.06                     | 0.44              |
| 22:DA:881:G:C2     | 22:DA:882:G:N7    | 2.85                     | 0.44              |
| 26:DE:76:PRO:HA    | 26:DE:82:GLY:HA2  | 1.98                     | 0.44              |
| 30:DI:93:PRO:HB3   | 30:DI:136:MET:HA  | 1.99                     | 0.44              |
| 31:DJ:6:ALA:O      | 31:DJ:7:LYS:CG    | 2.65                     | 0.44              |
| 33:DL:96:LYS:HD3   | 33:DL:103:ILE:HA  | 1.98                     | 0.44              |
| 33:DL:116:VAL:HG21 | 33:DL:135:ILE:HA  | 1.99                     | 0.44              |
| 35:DN:48:VAL:N     | 35:DN:50:PRO:HD2  | 2.33                     | 0.44              |
| 42:DU:44:LYS:HE3   | 42:DU:46:GLN:CB   | 2.48                     | 0.44              |
| 44:DW:45:PHE:HB3   | 44:DW:80:ILE:CD1  | 2.47                     | 0.44              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 45:DX:21:ALA:O    | 45:DX:22:LEU:HB2   | 2.17                     | 0.44              |
| 1:AA:1050:G:C2    | 1:AA:1209:C:O2     | 2.69                     | 0.44              |
| 1:AA:1500:A:OP2   | 1:AA:1505:G:OP1    | 2.35                     | 0.44              |
| 1:AA:394:G:C5     | 1:AA:395:C:C5      | 3.05                     | 0.44              |
| 1:AA:815:A:N7     | 1:AA:1509:C:O2'    | 2.49                     | 0.44              |
| 1:AA:844:G:N3     | 1:AA:845:A:C8      | 2.85                     | 0.44              |
| 2:AB:15:HIS:O     | 2:AB:16:PHE:C      | 2.55                     | 0.44              |
| 2:AB:70:VAL:O     | 2:AB:163:VAL:HA    | 2.17                     | 0.44              |
| 4:AD:122:ALA:O    | 4:AD:123:ILE:HG23  | 2.16                     | 0.44              |
| 7:AG:8:GLY:O      | 7:AG:9:GLN:HB3     | 2.17                     | 0.44              |
| 9:AI:25:ASN:HB2   | 9:AI:27:LYS:HG2    | 1.98                     | 0.44              |
| 11:AK:29:ASN:OD1  | 11:AK:47:ALA:HB3   | 2.18                     | 0.44              |
| 1:AA:980:C:O3'    | 14:AN:13:ARG:NH2   | 2.50                     | 0.44              |
| 14:AN:26:GLU:HG2  | 14:AN:27:LEU:N     | 2.30                     | 0.44              |
| 14:AN:47:LYS:HD2  | 19:AS:13:LEU:HD21  | 1.99                     | 0.44              |
| 15:AO:55:GLY:O    | 15:AO:58:ARG:HB3   | 2.17                     | 0.44              |
| 16:AP:20:VAL:HG23 | 16:AP:34:GLU:O     | 2.18                     | 0.44              |
| 49:B1:40:ASP:C    | 49:B1:40:ASP:OD1   | 2.55                     | 0.44              |
| 49:B1:17:THR:HG21 | 49:B1:42:VAL:HB    | 1.98                     | 0.44              |
| 53:B5:65:LEU:CD2  | 53:B5:195:ARG:CB   | 2.95                     | 0.44              |
| 22:BA:1071:G:P    | 22:BA:1071:G:H8    | 2.39                     | 0.44              |
| 22:BA:1073:A:C2'  | 22:BA:1074:G:H5''  | 2.47                     | 0.44              |
| 22:BA:1503:A:C6   | 22:BA:1504:A:C5    | 3.05                     | 0.44              |
| 22:BA:1718:G:C2   | 22:BA:1719:G:C8    | 3.06                     | 0.44              |
| 22:BA:1709:U:C2   | 22:BA:1750:G:N2    | 2.85                     | 0.44              |
| 22:BA:1988:G:H2'  | 22:BA:1989:G:O4'   | 2.17                     | 0.44              |
| 22:BA:2627:G:C6   | 22:BA:2628:C:C4    | 3.06                     | 0.44              |
| 22:BA:440:C:C2'   | 22:BA:441:U:H5'    | 2.47                     | 0.44              |
| 22:BA:878:A:H5'   | 22:BA:879:G:OP2    | 2.17                     | 0.44              |
| 25:BD:142:VAL:HB  | 25:BD:143:PRO:CD   | 2.47                     | 0.44              |
| 26:BE:197:GLU:O   | 26:BE:201:ALA:N    | 2.50                     | 0.44              |
| 29:BH:100:ALA:HB2 | 29:BH:115:VAL:HG21 | 1.98                     | 0.44              |
| 29:BH:62:LEU:O    | 29:BH:62:LEU:HD12  | 2.17                     | 0.44              |
| 35:BN:55:ALA:HA   | 35:BN:80:PHE:CE1   | 2.53                     | 0.44              |
| 36:BO:12:THR:O    | 36:BO:12:THR:HG22  | 2.16                     | 0.44              |
| 36:BO:79:ALA:CB   | 36:BO:113:ALA:HB3  | 2.47                     | 0.44              |
| 40:BS:55:ILE:CG2  | 40:BS:66:ILE:HG12  | 2.48                     | 0.44              |
| 44:BW:37:ILE:HD11 | 44:BW:61:ALA:HB2   | 1.98                     | 0.44              |
| 1:CA:1142:G:H5'   | 1:CA:1143:G:OP2    | 2.17                     | 0.44              |
| 1:CA:1491:G:C6    | 1:CA:1492:A:C6     | 3.05                     | 0.44              |
| 1:CA:734:G:C5     | 1:CA:735:C:C5      | 3.05                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:CB:18:HIS:O     | 2:CB:19:GLN:CB    | 2.65                     | 0.44              |
| 3:CC:196:ILE:O    | 3:CC:196:ILE:HG22 | 2.17                     | 0.44              |
| 4:CD:160:GLU:O    | 4:CD:163:GLU:CB   | 2.65                     | 0.44              |
| 5:CE:70:ASN:OD1   | 5:CE:70:ASN:N     | 2.49                     | 0.44              |
| 6:CF:45:ARG:HG2   | 6:CF:46:GLN:N     | 2.32                     | 0.44              |
| 9:CI:54:LEU:O     | 9:CI:55:VAL:HG13  | 2.18                     | 0.44              |
| 9:CI:95:ARG:HG2   | 9:CI:104:VAL:HG11 | 1.99                     | 0.44              |
| 10:CJ:52:LEU:HD23 | 10:CJ:62:ARG:HG2  | 1.99                     | 0.44              |
| 17:CQ:55:ILE:C    | 17:CQ:55:ILE:HD13 | 2.37                     | 0.44              |
| 22:DA:1070:A:H2'  | 22:DA:1097:U:O5'  | 2.17                     | 0.44              |
| 22:DA:1395:A:H2'  | 22:DA:1397:U:OP2  | 2.17                     | 0.44              |
| 22:DA:1435:G:O2'  | 22:DA:1436:G:H5'  | 2.17                     | 0.44              |
| 22:DA:1582:C:H2'  | 22:DA:1583:A:O4'  | 2.17                     | 0.44              |
| 22:DA:1663:G:C6   | 22:DA:1992:G:N7   | 2.86                     | 0.44              |
| 22:DA:1668:A:N3   | 22:DA:1674:G:C8   | 2.85                     | 0.44              |
| 22:DA:167:A:C2    | 22:DA:168:G:H1'   | 2.52                     | 0.44              |
| 22:DA:2038:G:N7   | 22:DA:2039:U:C5   | 2.86                     | 0.44              |
| 22:DA:2053:G:H2'  | 22:DA:2054:A:O4'  | 2.17                     | 0.44              |
| 22:DA:2114:A:C4   | 22:DA:2167:U:H4'  | 2.53                     | 0.44              |
| 22:DA:2440:C:N3   | 22:DA:2441:U:H1'  | 2.33                     | 0.44              |
| 22:DA:2695:U:O2   | 22:DA:2696:U:C5   | 2.71                     | 0.44              |
| 22:DA:607:U:H5    | 22:DA:619:G:C4    | 2.35                     | 0.44              |
| 22:DA:771:G:H2'   | 22:DA:771:G:N3    | 2.32                     | 0.44              |
| 22:DA:777:G:N2    | 22:DA:778:G:N9    | 2.66                     | 0.44              |
| 22:DA:997:G:OP1   | 38:DQ:92:ARG:NE   | 2.50                     | 0.44              |
| 22:DA:1797:G:H4'  | 24:DC:255:LYS:O   | 2.18                     | 0.44              |
| 27:DF:169:LEU:O   | 27:DF:169:LEU:HG  | 2.16                     | 0.44              |
| 29:DH:1:MET:CE    | 29:DH:27:ARG:NH1  | 2.80                     | 0.44              |
| 29:DH:37:VAL:HG22 | 29:DH:38:PRO:HD2  | 1.98                     | 0.44              |
| 32:DK:34:GLY:O    | 32:DK:35:VAL:C    | 2.54                     | 0.44              |
| 22:DA:2334:U:O3'  | 36:DO:13:ARG:HD3  | 2.17                     | 0.44              |
| 38:DQ:10:ALA:C    | 38:DQ:12:ALA:N    | 2.71                     | 0.44              |
| 1:AA:1154:G:C2    | 1:AA:1155:A:N7    | 2.85                     | 0.44              |
| 1:AA:1251:A:H2'   | 1:AA:1252:A:C8    | 2.53                     | 0.44              |
| 1:AA:189:A:C6     | 1:AA:190:A:N1     | 2.85                     | 0.44              |
| 1:AA:510:A:H5''   | 1:AA:511:C:OP1    | 2.18                     | 0.44              |
| 1:AA:833:G:N2     | 1:AA:834:U:H1'    | 2.32                     | 0.44              |
| 2:AB:32:PHE:C     | 2:AB:32:PHE:CD1   | 2.90                     | 0.44              |
| 3:AC:84:VAL:CG1   | 3:AC:101:ILE:CG2  | 2.95                     | 0.44              |
| 4:AD:126:ASN:HA   | 4:AD:142:VAL:HG23 | 2.00                     | 0.44              |
| 4:AD:90:LEU:C     | 4:AD:90:LEU:HD12  | 2.38                     | 0.44              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 7:AG:56:LYS:O      | 7:AG:57:SER:OG    | 2.29                     | 0.44              |
| 7:AG:80:VAL:O      | 7:AG:81:GLY:C     | 2.56                     | 0.44              |
| 10:AJ:5:ARG:HG2    | 10:AJ:79:PRO:HG3  | 1.99                     | 0.44              |
| 12:AL:44:LYS:O     | 12:AL:45:PRO:C    | 2.55                     | 0.44              |
| 12:AL:73:ASN:O     | 12:AL:74:LEU:CD2  | 2.65                     | 0.44              |
| 1:AA:750:C:O2'     | 15:AO:21:ASP:HA   | 2.17                     | 0.44              |
| 18:AR:71:THR:OG1   | 18:AR:73:ARG:HB2  | 2.18                     | 0.44              |
| 19:AS:29:LYS:CB    | 19:AS:30:PRO:HD2  | 2.47                     | 0.44              |
| 20:AT:71:LYS:HD2   | 20:AT:74:ARG:HH21 | 1.80                     | 0.44              |
| 20:AT:74:ARG:O     | 20:AT:78:ASN:OD1  | 2.34                     | 0.44              |
| 18:AR:35:GLU:OE2   | 21:AU:5:LYS:HE3   | 2.18                     | 0.44              |
| 49:B1:29:THR:O     | 49:B1:31:PRO:CD   | 2.66                     | 0.44              |
| 49:B1:34:LEU:H     | 49:B1:52:ALA:HB2  | 1.82                     | 0.44              |
| 22:BA:1128:G:O4'   | 22:BA:2516:A:O2'  | 2.35                     | 0.44              |
| 22:BA:1421:G:N2    | 22:BA:1495:A:N1   | 2.65                     | 0.44              |
| 22:BA:1501:G:C2'   | 22:BA:1502:A:H5'  | 2.48                     | 0.44              |
| 22:BA:1846:G:N2    | 22:BA:1895:C:C2   | 2.86                     | 0.44              |
| 22:BA:225:C:H2'    | 22:BA:226:A:O4'   | 2.17                     | 0.44              |
| 22:BA:2779:U:C6    | 22:BA:2781:A:C2   | 3.06                     | 0.44              |
| 22:BA:2846:G:H2'   | 22:BA:2847:U:O4'  | 2.18                     | 0.44              |
| 22:BA:2856:A:N6    | 22:BA:2857:G:C6   | 2.85                     | 0.44              |
| 22:BA:482:A:C5'    | 22:BA:483:A:OP1   | 2.66                     | 0.44              |
| 22:BA:612:G:H2'    | 22:BA:614:A:C8    | 2.51                     | 0.44              |
| 28:BG:121:ILE:HG22 | 28:BG:122:THR:N   | 2.32                     | 0.44              |
| 28:BG:85:LYS:HG3   | 28:BG:141:ILE:CD1 | 2.47                     | 0.44              |
| 29:BH:31:VAL:N     | 29:BH:32:PRO:CD   | 2.80                     | 0.44              |
| 30:BI:62:TYR:CD2   | 30:BI:62:TYR:N    | 2.84                     | 0.44              |
| 35:BN:32:GLU:CD    | 35:BN:86:ARG:HH22 | 2.20                     | 0.44              |
| 36:BO:78:VAL:HG23  | 36:BO:79:ALA:N    | 2.32                     | 0.44              |
| 37:BP:53:ARG:HG2   | 37:BP:53:ARG:HH11 | 1.81                     | 0.44              |
| 40:BS:37:THR:HG22  | 40:BS:38:TYR:CE1  | 2.53                     | 0.44              |
| 47:BZ:24:LEU:HD11  | 47:BZ:54:MET:CE   | 2.48                     | 0.44              |
| 1:CA:1029:U:O2     | 1:CA:1031:C:H1'   | 2.18                     | 0.44              |
| 1:CA:1138:G:C2     | 1:CA:1140:C:C4    | 3.06                     | 0.44              |
| 1:CA:1160:G:O6     | 1:CA:1181:G:C6    | 2.70                     | 0.44              |
| 1:CA:130:A:OP1     | 17:CQ:65:ARG:HD2  | 2.18                     | 0.44              |
| 1:CA:174:A:C4      | 1:CA:175:C:C6     | 3.05                     | 0.44              |
| 1:CA:144:G:C5      | 1:CA:179:A:C2     | 3.06                     | 0.44              |
| 1:CA:505:G:H5'     | 1:CA:534:U:C2     | 2.53                     | 0.44              |
| 1:CA:68:G:C5       | 1:CA:69:G:H1'     | 2.52                     | 0.44              |
| 1:CA:747:A:C5      | 1:CA:748:G:C5     | 3.05                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:765:G:H5''    | 1:CA:766:A:OP1     | 2.17                     | 0.44              |
| 1:CA:853:C:H2'     | 1:CA:854:U:O4'     | 2.18                     | 0.44              |
| 1:CA:862:C:C2      | 1:CA:863:U:C5      | 3.05                     | 0.44              |
| 1:CA:888:G:H4'     | 1:CA:1488:G:O2'    | 2.17                     | 0.44              |
| 5:CE:103:THR:O     | 5:CE:122:ASN:HA    | 2.18                     | 0.44              |
| 1:CA:824:G:H1'     | 8:CH:2:SER:HA      | 2.00                     | 0.44              |
| 14:CN:93:ILE:HG21  | 14:CN:96:LEU:HD22  | 1.99                     | 0.44              |
| 15:CO:58:ARG:O     | 15:CO:62:GLN:HB2   | 2.18                     | 0.44              |
| 16:CP:5:ARG:O      | 16:CP:19:VAL:HA    | 2.17                     | 0.44              |
| 20:CT:67:ILE:O     | 20:CT:68:HIS:O     | 2.34                     | 0.44              |
| 20:CT:72:ALA:O     | 20:CT:75:HIS:HB2   | 2.18                     | 0.44              |
| 21:CU:34:ARG:HD3   | 21:CU:35:ARG:CB    | 2.48                     | 0.44              |
| 48:D0:7:LYS:HE2    | 48:D0:8:PRO:O      | 2.17                     | 0.44              |
| 52:D4:17:VAL:HG11  | 52:D4:26:ILE:HD13  | 1.99                     | 0.44              |
| 22:DA:1194:A:H2'   | 22:DA:1195:G:O5'   | 2.18                     | 0.44              |
| 22:DA:158:U:C2'    | 22:DA:159:G:H5'    | 2.46                     | 0.44              |
| 22:DA:1655:A:C6    | 22:DA:1656:C:C2    | 3.05                     | 0.44              |
| 22:DA:2051:A:N3    | 22:DA:2052:A:N6    | 2.61                     | 0.44              |
| 22:DA:2221:G:C5    | 22:DA:2222:C:C5    | 3.05                     | 0.44              |
| 22:DA:2238:G:H4'   | 22:DA:2239:G:OP1   | 2.17                     | 0.44              |
| 22:DA:248:G:O2'    | 22:DA:2432:A:OP1   | 2.23                     | 0.44              |
| 22:DA:2652:C:N4    | 22:DA:2653:U:C4    | 2.85                     | 0.44              |
| 22:DA:2854:G:N2    | 22:DA:2864:G:N3    | 2.66                     | 0.44              |
| 22:DA:425:G:N1     | 22:DA:426:C:C4     | 2.85                     | 0.44              |
| 22:DA:41:C:H2'     | 22:DA:42:A:C8      | 2.52                     | 0.44              |
| 22:DA:503:A:C6     | 22:DA:506:G:C6     | 3.05                     | 0.44              |
| 22:DA:841:G:H2'    | 22:DA:842:U:O4'    | 2.18                     | 0.44              |
| 23:DB:48:U:H2'     | 23:DB:49:C:C6      | 2.52                     | 0.44              |
| 25:DD:112:THR:O    | 25:DD:112:THR:HG22 | 2.16                     | 0.44              |
| 25:DD:148:GLN:HB2  | 25:DD:152:PRO:HG2  | 2.00                     | 0.44              |
| 26:DE:48:THR:OG1   | 26:DE:49:ARG:N     | 2.50                     | 0.44              |
| 28:DG:167:GLU:HG3  | 28:DG:169:VAL:HG23 | 1.98                     | 0.44              |
| 29:DH:25:TYR:O     | 29:DH:29:PHE:HB3   | 2.18                     | 0.44              |
| 31:DJ:35:ARG:HB3   | 31:DJ:54:ILE:HD11  | 1.99                     | 0.44              |
| 33:DL:78:ARG:CZ    | 33:DL:113:ALA:HB1  | 2.48                     | 0.44              |
| 33:DL:17:LYS:HB3   | 33:DL:19:LEU:HD12  | 1.98                     | 0.44              |
| 33:DL:29:LYS:O     | 33:DL:30:THR:CB    | 2.64                     | 0.44              |
| 36:DO:18:LEU:O     | 36:DO:22:GLY:N     | 2.50                     | 0.44              |
| 22:DA:580:U:H4'    | 38:DQ:31:VAL:HG11  | 2.00                     | 0.44              |
| 42:DU:103:ILE:HG22 | 42:DU:103:ILE:O    | 2.16                     | 0.44              |
| 42:DU:83:VAL:HG11  | 42:DU:94:ARG:HD2   | 1.99                     | 0.44              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:AA:223:A:C4      | 1:AA:224:U:C5     | 3.05                     | 0.44              |
| 1:AA:471:U:H2'     | 1:AA:472:U:O4'    | 2.18                     | 0.44              |
| 1:AA:568:G:N3      | 1:AA:569:C:C6     | 2.85                     | 0.44              |
| 2:AB:125:THR:O     | 2:AB:126:PHE:HB3  | 2.17                     | 0.44              |
| 2:AB:132:LYS:HA    | 2:AB:132:LYS:HE3  | 1.99                     | 0.44              |
| 4:AD:105:MET:HG2   | 4:AD:171:LEU:HD22 | 1.98                     | 0.44              |
| 5:AE:80:THR:OG1    | 5:AE:81:LEU:N     | 2.51                     | 0.44              |
| 6:AF:38:ARG:HD2    | 6:AF:40:GLU:OE2   | 2.17                     | 0.44              |
| 10:AJ:35:GLN:OE1   | 10:AJ:35:GLN:HA   | 2.17                     | 0.44              |
| 11:AK:22:HIS:N     | 11:AK:33:THR:O    | 2.50                     | 0.44              |
| 12:AL:74:LEU:HD11  | 12:AL:80:ILE:HG21 | 2.00                     | 0.44              |
| 14:AN:7:LYS:O      | 14:AN:10:GLU:N    | 2.50                     | 0.44              |
| 15:AO:43:PHE:HB3   | 15:AO:53:ARG:NH2  | 2.31                     | 0.44              |
| 20:AT:67:ILE:CD1   | 20:AT:71:LYS:HG2  | 2.47                     | 0.44              |
| 21:AU:40:LYS:N     | 21:AU:41:PRO:HD2  | 2.32                     | 0.44              |
| 21:AU:53:VAL:O     | 21:AU:54:LYS:CB   | 2.66                     | 0.44              |
| 48:B0:27:SER:O     | 48:B0:28:LEU:C    | 2.56                     | 0.44              |
| 22:BA:1050:A:H2'   | 22:BA:1051:G:O4'  | 2.17                     | 0.44              |
| 22:BA:1444:G:H2'   | 22:BA:1445:G:C8   | 2.52                     | 0.44              |
| 22:BA:1793:C:O2'   | 22:BA:1794:A:H5'  | 2.18                     | 0.44              |
| 22:BA:1858:A:H1'   | 22:BA:1885:A:C2   | 2.53                     | 0.44              |
| 22:BA:1883:U:O4    | 22:BA:1884:G:N1   | 2.51                     | 0.44              |
| 22:BA:2345:G:H4'   | 22:BA:2346:A:H5'' | 1.99                     | 0.44              |
| 22:BA:2379:G:O3'   | 36:BO:17:LYS:NZ   | 2.49                     | 0.44              |
| 22:BA:412:A:H2'    | 22:BA:413:C:H5'   | 1.99                     | 0.44              |
| 22:BA:55:G:N3      | 22:BA:56:A:C8     | 2.86                     | 0.44              |
| 22:BA:581:C:H2'    | 22:BA:582:A:H8    | 1.83                     | 0.44              |
| 22:BA:599:A:O2'    | 22:BA:600:G:H5'   | 2.18                     | 0.44              |
| 23:BB:112:G:H2'    | 23:BB:113:C:C6    | 2.52                     | 0.44              |
| 23:BB:15:A:O2'     | 23:BB:16:G:OP1    | 2.35                     | 0.44              |
| 23:BB:3:C:C4       | 23:BB:4:C:C5      | 3.05                     | 0.44              |
| 24:BC:124:ILE:HG22 | 24:BC:124:ILE:O   | 2.17                     | 0.44              |
| 25:BD:106:LYS:HA   | 25:BD:175:LEU:O   | 2.18                     | 0.44              |
| 25:BD:85:ALA:O     | 25:BD:86:GLU:O    | 2.36                     | 0.44              |
| 22:BA:2311:A:H1'   | 27:BF:85:ILE:HD11 | 1.99                     | 0.44              |
| 33:BL:142:ILE:HG22 | 33:BL:142:ILE:O   | 2.17                     | 0.44              |
| 35:BN:33:ILE:HG23  | 35:BN:33:ILE:O    | 2.18                     | 0.44              |
| 36:BO:48:LEU:HD12  | 36:BO:87:ILE:CD1  | 2.46                     | 0.44              |
| 22:BA:1223:G:OP2   | 39:BR:68:ARG:NH1  | 2.50                     | 0.44              |
| 41:BT:16:VAL:O     | 41:BT:17:SER:CB   | 2.65                     | 0.44              |
| 1:CA:1007:U:C2'    | 1:CA:1008:U:C5'   | 2.95                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CA:1361:G:H3'   | 1:CA:1362:A:H5''  | 2.00                     | 0.44              |
| 1:CA:159:G:H5'    | 1:CA:160:A:OP2    | 2.18                     | 0.44              |
| 1:CA:230:G:H2'    | 1:CA:231:U:O4'    | 2.17                     | 0.44              |
| 1:CA:66:A:N6      | 1:CA:67:C:N4      | 2.65                     | 0.44              |
| 1:CA:73:C:HO2'    | 1:CA:74:A:P       | 2.39                     | 0.44              |
| 4:CD:148:LYS:H    | 4:CD:148:LYS:CE   | 2.31                     | 0.44              |
| 6:CF:91:ARG:HG2   | 6:CF:93:LYS:NZ    | 2.32                     | 0.44              |
| 7:CG:117:ALA:O    | 7:CG:121:ALA:CB   | 2.66                     | 0.44              |
| 7:CG:51:ALA:HB1   | 7:CG:57:SER:O     | 2.18                     | 0.44              |
| 8:CH:20:ALA:C     | 8:CH:22:LYS:H     | 2.21                     | 0.44              |
| 13:CM:6:GLY:O     | 13:CM:8:ASN:N     | 2.51                     | 0.44              |
| 14:CN:10:GLU:O    | 14:CN:13:ARG:N    | 2.51                     | 0.44              |
| 15:CO:37:ASN:O    | 15:CO:40:GLN:HB3  | 2.17                     | 0.44              |
| 17:CQ:46:VAL:HG12 | 17:CQ:47:HIS:N    | 2.33                     | 0.44              |
| 17:CQ:60:GLU:HB3  | 17:CQ:76:VAL:HG23 | 1.98                     | 0.44              |
| 11:CK:89:PRO:HD3  | 21:CU:29:LEU:HD11 | 1.97                     | 0.44              |
| 22:DA:1584:U:O2   | 22:DA:1584:U:H3'  | 2.17                     | 0.44              |
| 22:DA:2073:C:H5'' | 24:DC:228:VAL:CB  | 2.48                     | 0.44              |
| 22:DA:2502:G:H5'  | 22:DA:2503:A:C5'  | 2.47                     | 0.44              |
| 22:DA:226:A:H4'   | 22:DA:258:G:OP1   | 2.17                     | 0.44              |
| 22:DA:26:G:C6     | 22:DA:27:G:N1     | 2.86                     | 0.44              |
| 22:DA:749:A:C6    | 22:DA:750:A:N7    | 2.85                     | 0.44              |
| 22:DA:933:A:H5'   | 22:DA:934:U:OP2   | 2.18                     | 0.44              |
| 22:DA:2822:G:OP1  | 25:DD:164:GLN:NE2 | 2.48                     | 0.44              |
| 28:DG:133:LEU:CD1 | 28:DG:141:ILE:HB  | 2.47                     | 0.44              |
| 22:DA:2199:A:C1'  | 29:DH:28:ASN:ND2  | 2.80                     | 0.44              |
| 37:DP:60:THR:HA   | 37:DP:73:VAL:HA   | 1.99                     | 0.44              |
| 38:DQ:47:TYR:CD2  | 38:DQ:47:TYR:C    | 2.90                     | 0.44              |
| 44:DW:56:ASP:O    | 44:DW:57:HIS:HB2  | 2.16                     | 0.44              |
| 1:AA:946:A:C2     | 1:AA:1236:A:C2    | 3.06                     | 0.44              |
| 1:AA:279:A:H5''   | 1:AA:281:G:O4'    | 2.18                     | 0.44              |
| 1:AA:355:C:O2'    | 1:AA:388:G:N3     | 2.38                     | 0.44              |
| 1:AA:451:A:N6     | 1:AA:481:G:H5'    | 2.33                     | 0.44              |
| 1:AA:767:A:H2'    | 1:AA:768:A:O4'    | 2.17                     | 0.44              |
| 2:AB:67:ILE:O     | 2:AB:68:LEU:HB3   | 2.17                     | 0.44              |
| 3:AC:167:TRP:O    | 3:AC:168:TYR:HB2  | 2.16                     | 0.44              |
| 3:AC:114:LYS:HD3  | 3:AC:185:ASN:OD1  | 2.17                     | 0.44              |
| 4:AD:58:LYS:HD3   | 4:AD:203:LEU:CD2  | 2.48                     | 0.44              |
| 7:AG:69:VAL:HG23  | 7:AG:100:ALA:HB1  | 2.00                     | 0.44              |
| 9:AI:19:VAL:HA    | 9:AI:65:ILE:HG22  | 2.00                     | 0.44              |
| 14:AN:49:GLN:OE1  | 14:AN:49:GLN:CA   | 2.66                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:BA:1075:C:N3   | 22:BA:1076:C:N4   | 2.66                     | 0.44              |
| 22:BA:1356:G:C5   | 22:BA:1357:C:C5   | 3.05                     | 0.44              |
| 22:BA:1469:A:C2   | 22:BA:1470:A:C4   | 3.05                     | 0.44              |
| 22:BA:1811:G:C5   | 22:BA:1812:U:C5   | 3.06                     | 0.44              |
| 22:BA:1866:A:C6   | 22:BA:1876:A:N7   | 2.86                     | 0.44              |
| 22:BA:2040:G:H2'  | 22:BA:2041:U:O4'  | 2.17                     | 0.44              |
| 22:BA:2128:G:OP2  | 53:B5:37:LYS:HB2  | 2.18                     | 0.44              |
| 22:BA:2189:U:C2'  | 22:BA:2190:G:C1'  | 2.94                     | 0.44              |
| 22:BA:2191:A:C2   | 22:BA:2192:U:O4   | 2.71                     | 0.44              |
| 22:BA:2218:G:C2'  | 22:BA:2219:U:H5'  | 2.48                     | 0.44              |
| 22:BA:2366:A:H2'  | 22:BA:2367:G:O4'  | 2.17                     | 0.44              |
| 22:BA:2400:G:C2'  | 22:BA:2401:U:H5'  | 2.48                     | 0.44              |
| 22:BA:2503:A:N3   | 22:BA:2503:A:H5'  | 2.32                     | 0.44              |
| 22:BA:548:G:H4'   | 22:BA:549:G:N2    | 2.32                     | 0.44              |
| 22:BA:515:A:H1'   | 22:BA:581:C:H1'   | 2.00                     | 0.44              |
| 29:BH:97:ARG:O    | 29:BH:101:ASP:HB2 | 2.17                     | 0.44              |
| 29:BH:57:LYS:HG3  | 29:BH:58:LEU:N    | 2.33                     | 0.44              |
| 22:BA:826:U:O2'   | 33:BL:53:GLY:N    | 2.50                     | 0.44              |
| 36:BO:92:PHE:HB2  | 36:BO:117:PHE:CE1 | 2.52                     | 0.44              |
| 36:BO:40:ILE:HG22 | 36:BO:41:ALA:O    | 2.17                     | 0.44              |
| 41:BT:48:GLN:HG2  | 41:BT:53:VAL:O    | 2.18                     | 0.44              |
| 43:BV:63:ILE:HD12 | 43:BV:72:VAL:HG21 | 1.98                     | 0.44              |
| 44:BW:56:ASP:O    | 44:BW:57:HIS:CB   | 2.65                     | 0.44              |
| 1:CA:1004:A:H2'   | 1:CA:1005:A:C8    | 2.52                     | 0.44              |
| 1:CA:110:C:C4     | 1:CA:111:G:C5     | 3.06                     | 0.44              |
| 1:CA:1347:G:HO2'  | 1:CA:1348:U:P     | 2.38                     | 0.44              |
| 1:CA:862:C:H2'    | 1:CA:863:U:C6     | 2.52                     | 0.44              |
| 1:CA:954:G:N2     | 1:CA:1228:C:N3    | 2.65                     | 0.44              |
| 5:CE:11:LEU:HG    | 5:CE:12:GLN:N     | 2.33                     | 0.44              |
| 8:CH:104:VAL:HA   | 8:CH:126:ILE:CD1  | 2.48                     | 0.44              |
| 13:CM:81:MET:O    | 13:CM:82:ASP:C    | 2.56                     | 0.44              |
| 20:CT:67:ILE:HA   | 20:CT:67:ILE:HD13 | 1.84                     | 0.44              |
| 22:DA:116:C:H5'   | 22:DA:128:C:C5    | 2.53                     | 0.44              |
| 22:DA:117:G:N1    | 22:DA:119:A:N6    | 2.66                     | 0.44              |
| 22:DA:1355:G:C6   | 22:DA:1356:G:N7   | 2.85                     | 0.44              |
| 22:DA:153:U:H2'   | 22:DA:154:U:C6    | 2.52                     | 0.44              |
| 22:DA:1677:A:H5'' | 57:DA:3436:HOH:O  | 2.17                     | 0.44              |
| 22:DA:1734:G:C2   | 22:DA:1735:A:C5   | 3.06                     | 0.44              |
| 22:DA:2073:C:H5'' | 24:DC:228:VAL:HB  | 1.99                     | 0.44              |
| 22:DA:2121:G:C2   | 22:DA:2122:U:C2   | 3.06                     | 0.44              |
| 22:DA:2127:G:H1'  | 22:DA:2162:G:N7   | 2.33                     | 0.44              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:DA:2234:G:C4   | 22:DA:2235:G:C8    | 3.05                     | 0.44              |
| 22:DA:2347:C:O2'  | 49:D1:39:PHE:HB3   | 2.18                     | 0.44              |
| 22:DA:2392:A:OP2  | 51:D3:31:HIS:CE1   | 2.70                     | 0.44              |
| 22:DA:389:G:N9    | 22:DA:2413:G:H4'   | 2.32                     | 0.44              |
| 22:DA:2539:C:H4'  | 52:D4:3:VAL:HG11   | 1.99                     | 0.44              |
| 22:DA:2540:C:H2'  | 22:DA:2541:A:O4'   | 2.18                     | 0.44              |
| 22:DA:874:G:C2    | 22:DA:904:G:C2     | 3.05                     | 0.44              |
| 24:DC:3:VAL:CG1   | 24:DC:202:LEU:HD23 | 2.47                     | 0.44              |
| 31:DJ:35:ARG:HG2  | 31:DJ:40:HIS:NE2   | 2.33                     | 0.44              |
| 35:DN:65:LEU:HD11 | 35:DN:69:ARG:NH2   | 2.33                     | 0.44              |
| 36:DO:51:ALA:HB1  | 36:DO:77:ALA:HB1   | 2.00                     | 0.44              |
| 39:DR:68:ARG:HG3  | 39:DR:92:TRP:CZ3   | 2.52                     | 0.44              |
| 41:DT:2:ILE:HG23  | 41:DT:4:GLU:N      | 2.33                     | 0.44              |
| 41:DT:73:ARG:CZ   | 41:DT:73:ARG:HA    | 2.47                     | 0.44              |
| 44:DW:81:SER:O    | 44:DW:82:ILE:HG13  | 2.18                     | 0.44              |
| 46:DY:16:THR:O    | 46:DY:19:LEU:HB2   | 2.18                     | 0.44              |
| 47:DZ:52:SER:C    | 47:DZ:54:MET:H     | 2.20                     | 0.44              |
| 1:AA:1095:U:H2'   | 1:AA:1096:C:C6     | 2.53                     | 0.44              |
| 1:AA:1291:U:OP1   | 7:AG:38:THR:HG22   | 2.18                     | 0.44              |
| 1:AA:239:U:H5''   | 1:AA:240:G:OP2     | 2.18                     | 0.44              |
| 1:AA:949:A:C4     | 1:AA:950:U:C6      | 3.06                     | 0.44              |
| 1:AA:963:G:N3     | 1:AA:963:G:H2'     | 2.33                     | 0.44              |
| 1:AA:978:A:C4     | 1:AA:1319:A:C2     | 3.06                     | 0.44              |
| 2:AB:46:THR:CG2   | 2:AB:201:PRO:HB2   | 2.47                     | 0.44              |
| 7:AG:146:GLU:O    | 7:AG:149:LYS:HB2   | 2.16                     | 0.44              |
| 1:AA:973:G:H1'    | 10:AJ:56:HIS:CD2   | 2.52                     | 0.44              |
| 10:AJ:91:ASP:C    | 10:AJ:92:LEU:HG    | 2.37                     | 0.44              |
| 11:AK:53:ARG:O    | 11:AK:56:ARG:HG3   | 2.18                     | 0.44              |
| 11:AK:60:PRO:N    | 11:AK:91:PRO:HB2   | 2.33                     | 0.44              |
| 15:AO:2:SER:O     | 15:AO:3:LEU:HB3    | 2.18                     | 0.44              |
| 19:AS:42:PRO:C    | 19:AS:44:MET:H     | 2.20                     | 0.44              |
| 53:B5:214:TYR:O   | 53:B5:215:VAL:CB   | 2.65                     | 0.44              |
| 53:B5:61:GLY:O    | 53:B5:62:THR:C     | 2.55                     | 0.44              |
| 22:BA:1082:U:H5'  | 30:BI:119:GLY:N    | 2.33                     | 0.44              |
| 22:BA:1401:G:C6   | 22:BA:1402:U:C4    | 3.06                     | 0.44              |
| 22:BA:1536:C:O4'  | 22:BA:1537:G:C2    | 2.70                     | 0.44              |
| 22:BA:162:U:H4'   | 22:BA:163:C:OP1    | 2.17                     | 0.44              |
| 22:BA:1676:A:H2'  | 22:BA:1677:A:O4'   | 2.18                     | 0.44              |
| 22:BA:1734:G:H2'  | 22:BA:1735:A:O4'   | 2.18                     | 0.44              |
| 22:BA:2259:U:H1'  | 22:BA:2427:C:C2    | 2.52                     | 0.44              |
| 22:BA:1664:A:H1'  | 22:BA:2726:A:N1    | 2.33                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:BA:2880:C:N3    | 22:BA:2881:U:C5    | 2.86                     | 0.44              |
| 55:BA:3001:DOL:C37 | 55:BA:3001:DOL:C29 | 2.96                     | 0.44              |
| 22:BA:223:A:C5     | 22:BA:422:A:C8     | 3.06                     | 0.44              |
| 22:BA:630:G:H5''   | 22:BA:631:A:OP2    | 2.17                     | 0.44              |
| 28:BG:7:ALA:O      | 28:BG:69:ARG:NE    | 2.46                     | 0.44              |
| 29:BH:89:LYS:CE    | 29:BH:124:THR:HG22 | 2.48                     | 0.44              |
| 29:BH:4:ILE:HG23   | 29:BH:17:ASP:O     | 2.17                     | 0.44              |
| 36:BO:54:VAL:HG13  | 36:BO:54:VAL:O     | 2.17                     | 0.44              |
| 39:BR:14:VAL:CG1   | 39:BR:15:SER:N     | 2.80                     | 0.44              |
| 41:BT:2:ILE:N      | 41:BT:3:ARG:HB2    | 2.33                     | 0.44              |
| 42:BU:102:THR:HG22 | 42:BU:103:ILE:N    | 2.31                     | 0.44              |
| 43:BV:14:LYS:CD    | 43:BV:18:ARG:NH1   | 2.81                     | 0.44              |
| 43:BV:58:SER:O     | 43:BV:73:LYS:CE    | 2.66                     | 0.44              |
| 1:CA:1073:U:H2'    | 1:CA:1073:U:O2     | 2.17                     | 0.44              |
| 1:CA:1119:C:O2     | 1:CA:1155:A:C2     | 2.71                     | 0.44              |
| 1:CA:1149:C:C4     | 1:CA:1150:A:C6     | 3.05                     | 0.44              |
| 1:CA:1157:A:N6     | 1:CA:1178:G:H1'    | 2.32                     | 0.44              |
| 1:CA:121:U:C3'     | 1:CA:122:G:H5'     | 2.48                     | 0.44              |
| 1:CA:1126:U:N1     | 1:CA:1281:C:C5     | 2.86                     | 0.44              |
| 1:CA:1288:A:N6     | 1:CA:1289:A:N6     | 2.66                     | 0.44              |
| 1:CA:1304:G:O2'    | 1:CA:1333:A:N6     | 2.33                     | 0.44              |
| 1:CA:1492:A:N7     | 1:CA:1493:A:C2     | 2.86                     | 0.44              |
| 1:CA:260:G:C6      | 1:CA:261:U:C4      | 3.06                     | 0.44              |
| 1:CA:455:G:C2      | 1:CA:478:A:N1      | 2.86                     | 0.44              |
| 1:CA:483:C:H5''    | 1:CA:484:G:OP2     | 2.17                     | 0.44              |
| 1:CA:715:A:H1'     | 1:CA:777:A:C2      | 2.52                     | 0.44              |
| 1:CA:756:C:H2'     | 1:CA:757:U:H5'     | 2.00                     | 0.44              |
| 1:CA:791:G:C5      | 1:CA:792:A:N7      | 2.85                     | 0.44              |
| 1:CA:797:C:O2'     | 1:CA:798:U:H5'     | 2.18                     | 0.44              |
| 1:CA:803:G:C6      | 1:CA:804:U:N3      | 2.86                     | 0.44              |
| 1:CA:811:C:C5      | 1:CA:812:G:C5      | 3.06                     | 0.44              |
| 1:CA:834:U:C2      | 1:CA:835:U:C5      | 3.06                     | 0.44              |
| 1:CA:978:A:OP1     | 1:CA:1361:G:N2     | 2.42                     | 0.44              |
| 6:CF:70:VAL:HG23   | 6:CF:71:ILE:CD1    | 2.48                     | 0.44              |
| 7:CG:88:PRO:HD2    | 7:CG:151:PHE:O     | 2.17                     | 0.44              |
| 11:CK:56:ARG:O     | 11:CK:59:THR:HG23  | 2.17                     | 0.44              |
| 11:CK:30:THR:HG21  | 11:CK:92:GLY:HA3   | 1.99                     | 0.44              |
| 13:CM:43:VAL:O     | 13:CM:43:VAL:HG23  | 2.18                     | 0.44              |
| 15:CO:88:ARG:O     | 15:CO:88:ARG:HG3   | 2.18                     | 0.44              |
| 17:CQ:4:LYS:HG2    | 17:CQ:5:ILE:N      | 2.32                     | 0.44              |
| 22:DA:1255:U:C2'   | 22:DA:1256:G:OP1   | 2.66                     | 0.44              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 22:DA:1324:G:C1' | 22:DA:1616:A:N6   | 2.80                     | 0.44              |
| 22:DA:1420:A:C2  | 22:DA:2211:A:C4   | 3.05                     | 0.44              |
| 22:DA:1512:C:C4  | 22:DA:1513:U:C4   | 3.06                     | 0.44              |
| 22:DA:1768:C:H2' | 22:DA:1769:U:O4'  | 2.18                     | 0.44              |
| 22:DA:1926:U:H2' | 22:DA:1928:A:C8   | 2.53                     | 0.44              |
| 22:DA:1957:C:O2' | 22:DA:1985:C:H1'  | 2.18                     | 0.44              |
| 22:DA:2128:G:H1' | 22:DA:2173:A:O2'  | 2.17                     | 0.44              |
| 22:DA:2230:G:H5' | 45:DX:30:LEU:HD13 | 2.00                     | 0.44              |
| 22:DA:2341:G:C6  | 22:DA:2342:C:N3   | 2.86                     | 0.44              |
| 22:DA:2452:C:N4  | 22:DA:2453:A:N1   | 2.66                     | 0.44              |
| 22:DA:2602:A:H4' | 22:DA:2603:G:C5'  | 2.48                     | 0.44              |
| 22:DA:1638:C:C5' | 22:DA:2710:C:O2'  | 2.63                     | 0.44              |
| 22:DA:2744:G:N2  | 22:DA:2745:C:C2   | 2.86                     | 0.44              |
| 22:DA:2751:G:H4' | 28:DG:4:VAL:HG23  | 1.99                     | 0.44              |
| 22:DA:479:A:N3   | 22:DA:481:G:H5''  | 2.33                     | 0.44              |
| 22:DA:489:G:C2   | 22:DA:491:G:H1'   | 2.53                     | 0.44              |
| 22:DA:851:C:H2'  | 22:DA:852:U:C6    | 2.53                     | 0.44              |
| 24:DC:65:VAL:O   | 24:DC:67:PHE:CD1  | 2.71                     | 0.44              |
| 26:DE:8:ALA:HB2  | 26:DE:122:GLU:CG  | 2.48                     | 0.44              |
| 29:DH:31:VAL:CB  | 29:DH:32:PRO:HD3  | 2.47                     | 0.44              |
| 31:DJ:71:ASP:O   | 31:DJ:73:VAL:CG2  | 2.66                     | 0.44              |
| 32:DK:56:ASP:OD2 | 32:DK:56:ASP:N    | 2.51                     | 0.44              |
| 38:DQ:13:ARG:O   | 38:DQ:16:LYS:HB3  | 2.17                     | 0.44              |
| 39:DR:52:PRO:O   | 39:DR:53:PHE:HB2  | 2.18                     | 0.44              |
| 41:DT:37:ASP:CG  | 41:DT:38:ALA:N    | 2.70                     | 0.44              |
| 41:DT:91:GLN:O   | 41:DT:91:GLN:CG   | 2.66                     | 0.44              |
| 44:DW:45:PHE:HB3 | 44:DW:80:ILE:HD12 | 1.98                     | 0.44              |
| 1:AA:1030:U:OP2  | 1:AA:1031:C:C5    | 2.71                     | 0.44              |
| 1:AA:1244:G:C2   | 1:AA:1294:G:C2    | 3.06                     | 0.44              |
| 1:AA:194:C:C2'   | 1:AA:195:A:H5'    | 2.48                     | 0.44              |
| 1:AA:552:U:O2'   | 1:AA:553:A:H5'    | 2.17                     | 0.44              |
| 1:AA:569:C:H2'   | 1:AA:569:C:O2     | 2.17                     | 0.44              |
| 1:AA:85:U:O2     | 1:AA:85:U:O4'     | 2.36                     | 0.44              |
| 1:AA:981:U:C2    | 1:AA:982:U:C5     | 3.06                     | 0.44              |
| 2:AB:27:MET:CE   | 2:AB:193:PRO:HG3  | 2.48                     | 0.44              |
| 3:AC:77:ILE:HA   | 3:AC:84:VAL:CG2   | 2.48                     | 0.44              |
| 6:AF:17:GLN:O    | 6:AF:21:MET:HG3   | 2.18                     | 0.44              |
| 7:AG:55:GLY:C    | 7:AG:57:SER:H     | 2.21                     | 0.44              |
| 1:AA:1342:C:O2'  | 9:AI:126:GLN:CG   | 2.66                     | 0.44              |
| 11:AK:126:LYS:HA | 21:AU:34:ARG:HH21 | 1.82                     | 0.44              |
| 11:AK:63:ALA:CB  | 11:AK:92:GLY:HA3  | 2.48                     | 0.44              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 14:AN:90:ARG:HB2  | 14:AN:92:GLU:HG2  | 1.99                     | 0.44              |
| 17:AQ:14:SER:CB   | 17:AQ:22:VAL:CG1  | 2.94                     | 0.44              |
| 20:AT:44:LYS:HB3  | 20:AT:87:ALA:HB1  | 2.00                     | 0.44              |
| 20:AT:66:LEU:HD12 | 20:AT:66:LEU:C    | 2.38                     | 0.44              |
| 50:B2:35:ARG:NE   | 50:B2:42:LEU:HD21 | 2.33                     | 0.44              |
| 53:B5:66:PRO:HG3  | 53:B5:194:ILE:CB  | 2.48                     | 0.44              |
| 22:BA:1050:A:C2   | 22:BA:2751:G:C4   | 3.06                     | 0.44              |
| 22:BA:1056:G:O2'  | 22:BA:1086:A:H1'  | 2.18                     | 0.44              |
| 22:BA:1094:U:N3   | 22:BA:1097:U:OP2  | 2.50                     | 0.44              |
| 22:BA:136:G:C6    | 22:BA:137:U:O4    | 2.71                     | 0.44              |
| 22:BA:1394:U:H2'  | 22:BA:1395:A:O4'  | 2.17                     | 0.44              |
| 22:BA:1395:A:O2'  | 22:BA:1397:U:C6   | 2.67                     | 0.44              |
| 22:BA:1479:G:H2'  | 22:BA:1480:C:O4'  | 2.17                     | 0.44              |
| 22:BA:1492:G:C6   | 22:BA:1499:C:N3   | 2.86                     | 0.44              |
| 22:BA:1644:C:O2   | 22:BA:1644:C:H2'  | 2.17                     | 0.44              |
| 22:BA:1744:A:H2'  | 22:BA:1745:A:O4'  | 2.17                     | 0.44              |
| 22:BA:2191:A:C2   | 22:BA:2192:U:N3   | 2.86                     | 0.44              |
| 22:BA:263:G:C2'   | 22:BA:264:C:H5'   | 2.48                     | 0.44              |
| 22:BA:368:A:C6    | 22:BA:369:U:N3    | 2.86                     | 0.44              |
| 22:BA:616:A:C2    | 22:BA:617:G:H1'   | 2.52                     | 0.44              |
| 22:BA:863:A:O2'   | 22:BA:864:G:H5'   | 2.18                     | 0.44              |
| 26:BE:164:LEU:HB3 | 26:BE:167:VAL:HB  | 1.99                     | 0.44              |
| 27:BF:108:VAL:N   | 27:BF:109:PRO:HD2 | 2.33                     | 0.44              |
| 28:BG:153:ARG:O   | 28:BG:154:PRO:C   | 2.57                     | 0.44              |
| 36:BO:7:ARG:HG3   | 36:BO:96:GLY:HA3  | 1.99                     | 0.44              |
| 39:BR:66:HIS:CE1  | 39:BR:94:THR:HG22 | 2.53                     | 0.44              |
| 41:BT:1:MET:C     | 41:BT:2:ILE:HD12  | 2.38                     | 0.44              |
| 47:BZ:35:THR:HG22 | 47:BZ:36:VAL:N    | 2.32                     | 0.44              |
| 1:CA:1004:A:C6    | 1:CA:1005:A:N1    | 2.86                     | 0.44              |
| 1:CA:1077:G:N2    | 1:CA:1080:A:OP2   | 2.50                     | 0.44              |
| 1:CA:1197:A:C2'   | 1:CA:1198:G:H5'   | 2.47                     | 0.44              |
| 1:CA:960:U:O2'    | 1:CA:1223:C:H4'   | 2.17                     | 0.44              |
| 1:CA:147:G:C2     | 1:CA:148:G:C6     | 3.06                     | 0.44              |
| 1:CA:173:U:H3'    | 1:CA:174:A:H5'    | 1.99                     | 0.44              |
| 1:CA:327:A:C2     | 1:CA:329:A:C4     | 3.05                     | 0.44              |
| 1:CA:438:U:C2     | 1:CA:494:G:C6     | 3.06                     | 0.44              |
| 1:CA:711:G:N2     | 1:CA:712:A:C4     | 2.86                     | 0.44              |
| 1:CA:774:G:C5     | 1:CA:775:G:C8     | 3.06                     | 0.44              |
| 2:CB:104:TRP:CH2  | 2:CB:108:ARG:HD3  | 2.53                     | 0.44              |
| 2:CB:173:ILE:HG22 | 2:CB:177:ASN:ND2  | 2.33                     | 0.44              |
| 2:CB:93:ASN:OD1   | 2:CB:94:HIS:N     | 2.50                     | 0.44              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:CC:30:ALA:O    | 3:CC:34:ASP:HB2   | 2.18                     | 0.44              |
| 4:CD:188:ARG:NH2 | 4:CD:197:GLU:OE2  | 2.49                     | 0.44              |
| 4:CD:3:ARG:O     | 4:CD:5:LEU:HD13   | 2.18                     | 0.44              |
| 5:CE:156:LYS:O   | 5:CE:159:LYS:NZ   | 2.48                     | 0.44              |
| 6:CF:8:PHE:CD2   | 6:CF:8:PHE:N      | 2.86                     | 0.44              |
| 7:CG:71:PRO:HD2  | 7:CG:96:ARG:O     | 2.18                     | 0.44              |
| 9:CI:55:VAL:HG23 | 9:CI:55:VAL:O     | 2.17                     | 0.44              |
| 11:CK:126:LYS:O  | 21:CU:34:ARG:CZ   | 2.66                     | 0.44              |
| 12:CL:51:LYS:HD2 | 12:CL:51:LYS:N    | 2.33                     | 0.44              |
| 13:CM:25:VAL:O   | 13:CM:25:VAL:HG13 | 2.18                     | 0.44              |
| 13:CM:53:ILE:O   | 13:CM:57:ARG:HB2  | 2.17                     | 0.44              |
| 18:CR:37:GLY:O   | 18:CR:63:ARG:NH2  | 2.47                     | 0.44              |
| 19:CS:55:ARG:CZ  | 19:CS:79:THR:CG2  | 2.95                     | 0.44              |
| 20:CT:32:ILE:CG1 | 20:CT:54:MET:HE3  | 2.48                     | 0.44              |
| 21:CU:37:PHE:O   | 21:CU:39:GLU:N    | 2.44                     | 0.44              |
| 22:DA:117:G:C6   | 22:DA:119:A:N1    | 2.86                     | 0.44              |
| 22:DA:1287:A:H2' | 22:DA:1288:G:H5'  | 2.00                     | 0.44              |
| 22:DA:13:A:N3    | 22:DA:14:A:N6     | 2.61                     | 0.44              |
| 22:DA:137:U:H2'  | 22:DA:140:C:C2    | 2.53                     | 0.44              |
| 22:DA:1754:A:C6  | 22:DA:1755:A:C5   | 3.05                     | 0.44              |
| 22:DA:1809:A:H2' | 22:DA:1810:A:H8   | 1.78                     | 0.44              |
| 22:DA:1905:C:O4' | 22:DA:1928:A:C2   | 2.71                     | 0.44              |
| 22:DA:1906:G:C8  | 22:DA:1929:G:H2'  | 2.53                     | 0.44              |
| 22:DA:2106:U:H2' | 22:DA:2107:G:C8   | 2.53                     | 0.44              |
| 22:DA:2163:A:OP2 | 22:DA:2171:A:C8   | 2.71                     | 0.44              |
| 22:DA:2431:U:H2' | 22:DA:2433:A:OP2  | 2.17                     | 0.44              |
| 22:DA:2544:G:H5' | 22:DA:2645:G:C2   | 2.53                     | 0.44              |
| 22:DA:2837:A:H2' | 22:DA:2838:G:O4'  | 2.18                     | 0.44              |
| 22:DA:478:A:C6   | 22:DA:480:A:C6    | 3.06                     | 0.44              |
| 22:DA:560:C:O2   | 38:DQ:48:ARG:NH1  | 2.48                     | 0.44              |
| 22:DA:568:U:H2'  | 22:DA:570:G:OP2   | 2.17                     | 0.44              |
| 22:DA:772:C:N3   | 22:DA:773:U:C5    | 2.86                     | 0.44              |
| 22:DA:79:C:H2'   | 22:DA:346:A:N3    | 2.32                     | 0.44              |
| 22:DA:810:U:OP1  | 57:DA:3333:HOH:O  | 2.21                     | 0.44              |
| 22:DA:855:G:C2   | 22:DA:923:G:N3    | 2.86                     | 0.44              |
| 22:DA:8:C:O2'    | 22:DA:9:G:H5'     | 2.18                     | 0.44              |
| 26:DE:109:LEU:O  | 26:DE:112:LEU:HB2 | 2.17                     | 0.44              |
| 33:DL:22:GLY:O   | 33:DL:25:SER:OG   | 2.36                     | 0.44              |
| 34:DM:2:LEU:N    | 34:DM:2:LEU:HD12  | 2.33                     | 0.44              |
| 1:AA:125:U:H2'   | 1:AA:126:G:O4'    | 2.17                     | 0.44              |
| 1:AA:815:A:H4'   | 1:AA:817:C:C4     | 2.53                     | 0.44              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:AB:10:LEU:HD23  | 2:AB:10:LEU:C      | 2.38                     | 0.44              |
| 2:AB:101:LEU:CD1  | 2:AB:158:PRO:HG2   | 2.48                     | 0.44              |
| 4:AD:197:GLU:O    | 4:AD:199:LEU:N     | 2.50                     | 0.44              |
| 1:AA:933:G:OP2    | 7:AG:3:ARG:CB      | 2.66                     | 0.44              |
| 8:AH:111:MET:CE   | 8:AH:116:ALA:HA    | 2.44                     | 0.44              |
| 8:AH:39:VAL:CG1   | 8:AH:112:THR:HG22  | 2.48                     | 0.44              |
| 8:AH:49:PHE:HB3   | 8:AH:61:LEU:CD2    | 2.47                     | 0.44              |
| 9:AI:127:PHE:CD2  | 9:AI:127:PHE:C     | 2.91                     | 0.44              |
| 10:AJ:65:TYR:CB   | 14:AN:96:LEU:HD11  | 2.48                     | 0.44              |
| 10:AJ:66:GLU:HB3  | 14:AN:99:ALA:HB2   | 2.00                     | 0.44              |
| 14:AN:41:ARG:HD3  | 14:AN:42:TRP:CH2   | 2.53                     | 0.44              |
| 16:AP:56:ARG:O    | 16:AP:59:HIS:HB3   | 2.18                     | 0.44              |
| 17:AQ:48:ASP:CG   | 17:AQ:52:GLU:OE1   | 2.56                     | 0.44              |
| 17:AQ:5:ILE:N     | 17:AQ:5:ILE:HD12   | 2.33                     | 0.44              |
| 1:AA:1014:A:C2    | 19:AS:34:TRP:CZ2   | 3.06                     | 0.44              |
| 19:AS:50:ALA:HB1  | 19:AS:57:HIS:HB3   | 1.99                     | 0.44              |
| 1:AA:1539:C:H5''  | 21:AU:18:ARG:HG3   | 1.99                     | 0.44              |
| 49:B1:51:GLU:OE2  | 49:B1:53:LYS:HD3   | 2.18                     | 0.44              |
| 51:B3:32:ILE:O    | 51:B3:32:ILE:HG22  | 2.18                     | 0.44              |
| 22:BA:108:G:C5    | 22:BA:109:C:C5     | 3.06                     | 0.44              |
| 22:BA:1688:U:H1'  | 22:BA:1701:A:C5    | 2.52                     | 0.44              |
| 22:BA:1716:U:O2'  | 22:BA:1717:A:H5'   | 2.18                     | 0.44              |
| 22:BA:1951:U:H2'  | 22:BA:1953:A:OP2   | 2.18                     | 0.44              |
| 22:BA:608:A:C2    | 22:BA:609:A:N3     | 2.86                     | 0.44              |
| 22:BA:785:G:C6    | 22:BA:786:C:C4     | 3.05                     | 0.44              |
| 27:BF:36:LEU:HD11 | 27:BF:99:PHE:CZ    | 2.53                     | 0.44              |
| 27:BF:73:SER:OG   | 27:BF:80:ARG:HA    | 2.18                     | 0.44              |
| 29:BH:99:ILE:CD1  | 29:BH:117:LEU:HD13 | 2.48                     | 0.44              |
| 30:BI:58:VAL:HG12 | 30:BI:59:ILE:H     | 1.82                     | 0.44              |
| 35:BN:52:ILE:HG21 | 35:BN:94:TYR:CG    | 2.53                     | 0.44              |
| 40:BS:36:LEU:CD1  | 40:BS:48:LYS:HA    | 2.48                     | 0.44              |
| 40:BS:41:LYS:O    | 40:BS:43:ALA:N     | 2.50                     | 0.44              |
| 41:BT:49:LYS:HD3  | 41:BT:49:LYS:H     | 1.82                     | 0.44              |
| 42:BU:12:ILE:HG13 | 42:BU:21:LYS:O     | 2.18                     | 0.44              |
| 43:BV:10:LYS:H    | 43:BV:10:LYS:CE    | 2.31                     | 0.44              |
| 1:CA:1213:A:C5    | 1:CA:1215:G:C4     | 3.06                     | 0.44              |
| 1:CA:1345:U:H4'   | 1:CA:1346:A:H5'    | 1.99                     | 0.44              |
| 1:CA:1462:C:H2'   | 1:CA:1463:U:C6     | 2.53                     | 0.44              |
| 1:CA:1480:A:H2'   | 1:CA:1481:U:O4'    | 2.18                     | 0.44              |
| 1:CA:237:G:C4     | 1:CA:238:A:C8      | 3.06                     | 0.44              |
| 1:CA:246:A:N3     | 1:CA:279:A:N6      | 2.65                     | 0.44              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:CA:552:U:C2     | 1:CA:553:A:C8      | 3.05                     | 0.44              |
| 1:CA:73:C:O2'     | 1:CA:74:A:P        | 2.76                     | 0.44              |
| 1:CA:781:A:OP2    | 57:CA:1812:HOH:O   | 2.21                     | 0.44              |
| 4:CD:149:ALA:O    | 4:CD:152:GLN:HB2   | 2.17                     | 0.44              |
| 8:CH:51:VAL:HG22  | 8:CH:51:VAL:O      | 2.18                     | 0.44              |
| 11:CK:67:ALA:HB1  | 11:CK:100:LEU:HD13 | 2.00                     | 0.44              |
| 11:CK:118:HIS:O   | 11:CK:119:ASN:HB2  | 2.18                     | 0.44              |
| 12:CL:51:LYS:N    | 12:CL:51:LYS:CD    | 2.81                     | 0.44              |
| 13:CM:85:CYS:HB3  | 19:CS:74:PHE:CE2   | 2.52                     | 0.44              |
| 22:DA:110:G:N3    | 22:DA:110:G:H2'    | 2.33                     | 0.44              |
| 22:DA:1780:A:OP1  | 57:DA:3687:HOH:O   | 2.20                     | 0.44              |
| 22:DA:1829:A:H2'  | 24:DC:15:HIS:NE2   | 2.33                     | 0.44              |
| 22:DA:2199:A:C4   | 22:DA:2225:A:N1    | 2.86                     | 0.44              |
| 22:DA:2728:U:C2   | 22:DA:2729:G:C8    | 3.06                     | 0.44              |
| 22:DA:39:G:N2     | 22:DA:441:U:C2     | 2.86                     | 0.44              |
| 22:DA:483:A:O2'   | 42:DU:56:GLY:HA3   | 2.18                     | 0.44              |
| 22:DA:546:U:O2    | 22:DA:546:U:C2'    | 2.65                     | 0.44              |
| 23:DB:34:A:N6     | 23:DB:44:G:O2'     | 2.48                     | 0.44              |
| 23:DB:21:G:N2     | 23:DB:63:C:C2      | 2.86                     | 0.44              |
| 24:DC:247:PRO:HG2 | 24:DC:248:TRP:CZ3  | 2.53                     | 0.44              |
| 25:DD:105:LYS:O   | 25:DD:177:VAL:HG12 | 2.18                     | 0.44              |
| 22:DA:2784:U:H4'  | 25:DD:42:ASN:O     | 2.18                     | 0.44              |
| 35:DN:51:LEU:N    | 35:DN:51:LEU:CD2   | 2.79                     | 0.44              |
| 35:DN:80:PHE:O    | 35:DN:85:PRO:HD3   | 2.18                     | 0.44              |
| 42:DU:71:ALA:HB3  | 42:DU:80:ALA:HB1   | 1.98                     | 0.44              |
| 44:DW:71:VAL:HA   | 44:DW:77:ARG:O     | 2.17                     | 0.44              |
| 1:AA:1048:G:N3    | 1:AA:1050:G:N7     | 2.65                     | 0.43              |
| 1:AA:1077:G:N1    | 1:AA:1081:A:C6     | 2.85                     | 0.43              |
| 1:AA:1136:C:OP2   | 1:AA:1137:C:C5     | 2.71                     | 0.43              |
| 1:AA:1130:A:C2    | 1:AA:1146:A:C5     | 3.06                     | 0.43              |
| 1:AA:1197:A:OP1   | 1:AA:1198:G:OP2    | 2.36                     | 0.43              |
| 1:AA:126:G:OP1    | 1:AA:605:U:O2'     | 2.28                     | 0.43              |
| 1:AA:263:A:H2'    | 1:AA:264:C:C5      | 2.53                     | 0.43              |
| 1:AA:495:A:C2     | 1:AA:496:A:C6      | 3.05                     | 0.43              |
| 2:AB:144:LEU:N    | 2:AB:144:LEU:HD23  | 2.32                     | 0.43              |
| 2:AB:78:GLU:HA    | 2:AB:81:LYS:HB3    | 2.00                     | 0.43              |
| 2:AB:99:GLY:O     | 2:AB:103:ASN:N     | 2.48                     | 0.43              |
| 4:AD:112:ALA:O    | 4:AD:115:ARG:N     | 2.50                     | 0.43              |
| 4:AD:145:ILE:HD12 | 4:AD:145:ILE:N     | 2.33                     | 0.43              |
| 8:AH:49:PHE:CB    | 8:AH:61:LEU:HD23   | 2.48                     | 0.43              |
| 8:AH:46:ILE:HG22  | 8:AH:63:LEU:HA     | 2.00                     | 0.43              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 9:AI:80:ARG:C      | 9:AI:80:ARG:HD2     | 2.37                     | 0.43              |
| 11:AK:34:ILE:HG13  | 11:AK:70:CYS:SG     | 2.58                     | 0.43              |
| 10:AJ:49:PHE:CD2   | 14:AN:77:PHE:CE1    | 3.05                     | 0.43              |
| 17:AQ:4:LYS:C      | 17:AQ:4:LYS:HD2     | 2.39                     | 0.43              |
| 17:AQ:81:LYS:C     | 17:AQ:83:VAL:N      | 2.69                     | 0.43              |
| 1:AA:1014:A:H5''   | 19:AS:14:HIS:CG     | 2.53                     | 0.43              |
| 22:BA:1303:G:O2'   | 22:BA:1304:A:H5'    | 2.17                     | 0.43              |
| 22:BA:1355:G:C2    | 22:BA:1356:G:C8     | 3.06                     | 0.43              |
| 22:BA:1851:U:C4    | 22:BA:1852:U:C4     | 3.06                     | 0.43              |
| 22:BA:1899:A:O2'   | 22:BA:1900:A:H5''   | 2.19                     | 0.43              |
| 22:BA:1949:G:C2    | 22:BA:1958:C:C2     | 3.05                     | 0.43              |
| 22:BA:2020:A:C2    | 22:BA:2022:U:O4'    | 2.70                     | 0.43              |
| 22:BA:2076:U:O5'   | 22:BA:2076:U:O2     | 2.36                     | 0.43              |
| 22:BA:22:C:C2'     | 22:BA:23:G:O5'      | 2.66                     | 0.43              |
| 22:BA:2506:U:C6    | 55:BA:3001:DOL:H422 | 2.52                     | 0.43              |
| 22:BA:996:A:N3     | 22:BA:997:G:C8      | 2.86                     | 0.43              |
| 23:BB:109:A:C5     | 23:BB:110:C:C4      | 3.06                     | 0.43              |
| 24:BC:125:LYS:HB2  | 24:BC:126:PRO:HD2   | 2.00                     | 0.43              |
| 24:BC:107:PRO:HB3  | 24:BC:142:HIS:HE1   | 1.82                     | 0.43              |
| 22:BA:1813:G:H1'   | 24:BC:50:THR:OG1    | 2.18                     | 0.43              |
| 27:BF:146:VAL:HG23 | 27:BF:146:VAL:O     | 2.18                     | 0.43              |
| 27:BF:69:LYS:N     | 27:BF:69:LYS:HD2    | 2.33                     | 0.43              |
| 28:BG:74:SER:HA    | 28:BG:77:ILE:CG1    | 2.48                     | 0.43              |
| 29:BH:89:LYS:HE3   | 29:BH:124:THR:HG22  | 1.99                     | 0.43              |
| 30:BI:38:PHE:O     | 30:BI:39:CYS:SG     | 2.76                     | 0.43              |
| 22:BA:2009:A:C4'   | 35:BN:107:ASN:HD22  | 2.30                     | 0.43              |
| 39:BR:39:LEU:C     | 39:BR:49:ILE:HG23   | 2.39                     | 0.43              |
| 42:BU:102:THR:CG2  | 42:BU:103:ILE:N     | 2.81                     | 0.43              |
| 43:BV:40:ILE:CG2   | 43:BV:41:GLU:N      | 2.81                     | 0.43              |
| 1:CA:1077:G:N2     | 1:CA:1081:A:C4      | 2.86                     | 0.43              |
| 1:CA:1238:A:H2'    | 1:CA:1241:G:H1'     | 1.99                     | 0.43              |
| 1:CA:1345:U:C2     | 1:CA:1377:A:N1      | 2.86                     | 0.43              |
| 1:CA:1493:A:H4'    | 22:DA:1913:A:N1     | 2.33                     | 0.43              |
| 1:CA:1537:U:C4     | 1:CA:1538:C:C4      | 3.06                     | 0.43              |
| 1:CA:35:G:C2       | 1:CA:550:G:C2       | 3.06                     | 0.43              |
| 1:CA:376:G:N3      | 1:CA:389:A:C2       | 2.86                     | 0.43              |
| 1:CA:378:G:N2      | 1:CA:386:C:O2       | 2.50                     | 0.43              |
| 1:CA:414:A:C6      | 1:CA:415:A:C5       | 3.05                     | 0.43              |
| 1:CA:458:U:H2'     | 1:CA:459:A:C8       | 2.53                     | 0.43              |
| 1:CA:57:G:C5       | 1:CA:58:C:C4        | 3.05                     | 0.43              |
| 1:CA:635:A:C5      | 1:CA:636:U:C5       | 3.06                     | 0.43              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:CA:971:G:N2      | 1:CA:1363:A:C8    | 2.86                     | 0.43              |
| 2:CB:60:ILE:HA     | 2:CB:63:ARG:HB2   | 2.00                     | 0.43              |
| 2:CB:68:LEU:CD2    | 2:CB:68:LEU:C     | 2.86                     | 0.43              |
| 3:CC:173:VAL:HG12  | 3:CC:173:VAL:O    | 2.18                     | 0.43              |
| 3:CC:23:PHE:CG     | 3:CC:24:ALA:N     | 2.85                     | 0.43              |
| 4:CD:129:VAL:O     | 4:CD:129:VAL:HG13 | 2.17                     | 0.43              |
| 1:CA:8:A:N6        | 4:CD:206:LYS:HG2  | 2.33                     | 0.43              |
| 13:CM:14:HIS:HB2   | 13:CM:17:ILE:CD1  | 2.48                     | 0.43              |
| 15:CO:23:GLY:O     | 15:CO:24:SER:C    | 2.57                     | 0.43              |
| 16:CP:19:VAL:HG12  | 16:CP:37:GLY:CA   | 2.48                     | 0.43              |
| 22:DA:1317:G:C5    | 22:DA:1318:U:C4   | 3.05                     | 0.43              |
| 22:DA:162:U:H4'    | 22:DA:163:C:OP1   | 2.18                     | 0.43              |
| 22:DA:1693:U:H4'   | 22:DA:1694:C:OP2  | 2.18                     | 0.43              |
| 22:DA:1801:A:N7    | 24:DC:262:ARG:NH2 | 2.66                     | 0.43              |
| 22:DA:2093:G:C2    | 22:DA:2094:A:C8   | 3.06                     | 0.43              |
| 22:DA:185:G:C5     | 22:DA:212:G:N2    | 2.85                     | 0.43              |
| 22:DA:2716:C:H2'   | 22:DA:2717:C:C6   | 2.52                     | 0.43              |
| 22:DA:466:A:N1     | 22:DA:795:C:O2'   | 2.44                     | 0.43              |
| 22:DA:704:G:O2'    | 22:DA:725:G:O6    | 2.36                     | 0.43              |
| 25:DD:104:VAL:HG23 | 25:DD:105:LYS:N   | 2.33                     | 0.43              |
| 28:DG:24:ILE:HD13  | 28:DG:72:LEU:HD21 | 2.00                     | 0.43              |
| 29:DH:127:GLU:CG   | 29:DH:144:VAL:O   | 2.65                     | 0.43              |
| 32:DK:91:SER:O     | 32:DK:92:GLU:C    | 2.56                     | 0.43              |
| 34:DM:97:GLN:O     | 34:DM:100:LYS:HB2 | 2.18                     | 0.43              |
| 34:DM:57:VAL:HG11  | 34:DM:105:MET:SD  | 2.57                     | 0.43              |
| 35:DN:1:MET:HE3    | 35:DN:1:MET:N     | 2.31                     | 0.43              |
| 39:DR:69:GLY:O     | 39:DR:70:GLU:C    | 2.56                     | 0.43              |
| 41:DT:61:LEU:CD1   | 41:DT:62:VAL:N    | 2.81                     | 0.43              |
| 1:AA:1129:C:H4'    | 1:AA:1130:A:OP1   | 2.18                     | 0.43              |
| 1:AA:1298:U:O4'    | 1:AA:1299:A:C2    | 2.71                     | 0.43              |
| 1:AA:174:A:C2      | 1:AA:175:C:H1'    | 2.54                     | 0.43              |
| 1:AA:69:G:N3       | 1:AA:69:G:H2'     | 2.33                     | 0.43              |
| 1:AA:531:U:H5''    | 3:AC:161:GLU:OE2  | 2.18                     | 0.43              |
| 4:AD:191:LEU:O     | 4:AD:192:SER:CB   | 2.66                     | 0.43              |
| 7:AG:24:ALA:O      | 7:AG:27:VAL:HG22  | 2.18                     | 0.43              |
| 8:AH:15:ARG:HB2    | 8:AH:75:ILE:CG2   | 2.48                     | 0.43              |
| 9:AI:57:MET:SD     | 9:AI:58:VAL:N     | 2.84                     | 0.43              |
| 10:AJ:12:ALA:HB2   | 10:AJ:96:VAL:HA   | 2.00                     | 0.43              |
| 14:AN:17:ALA:HA    | 14:AN:55:SER:O    | 2.18                     | 0.43              |
| 15:AO:48:LYS:O     | 15:AO:50:HIS:N    | 2.49                     | 0.43              |
| 17:AQ:16:LYS:C     | 17:AQ:17:MET:CE   | 2.86                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:BA:1010:A:N3   | 22:BA:1153:C:H1'  | 2.33                     | 0.43              |
| 22:BA:1340:U:H4'  | 22:BA:1341:G:OP2  | 2.18                     | 0.43              |
| 22:BA:1419:A:C4   | 22:BA:1421:G:C8   | 3.06                     | 0.43              |
| 22:BA:1449:G:C4   | 22:BA:1450:G:C8   | 3.06                     | 0.43              |
| 22:BA:2364:C:OP1  | 44:BW:55:ARG:NH1  | 2.50                     | 0.43              |
| 22:BA:2788:C:O2'  | 22:BA:2809:A:N3   | 2.38                     | 0.43              |
| 22:BA:479:A:H4'   | 22:BA:480:A:OP1   | 2.19                     | 0.43              |
| 22:BA:501:A:H5'   | 22:BA:502:A:OP2   | 2.18                     | 0.43              |
| 22:BA:927:A:H2'   | 22:BA:928:A:O4'   | 2.18                     | 0.43              |
| 24:BC:21:ASN:O    | 24:BC:24:LEU:HB2  | 2.18                     | 0.43              |
| 25:BD:12:THR:HG21 | 37:BP:9:GLU:OE2   | 2.19                     | 0.43              |
| 26:BE:124:PHE:C   | 26:BE:124:PHE:CD1 | 2.92                     | 0.43              |
| 22:BA:451:U:H4'   | 26:BE:47:LYS:NZ   | 2.32                     | 0.43              |
| 29:BH:1:MET:HE3   | 29:BH:23:ALA:HA   | 2.00                     | 0.43              |
| 31:BJ:32:LEU:O    | 31:BJ:36:LEU:HG   | 2.18                     | 0.43              |
| 40:BS:29:VAL:HG21 | 40:BS:69:LEU:HB3  | 2.00                     | 0.43              |
| 41:BT:12:ARG:HB2  | 41:BT:33:LYS:O    | 2.18                     | 0.43              |
| 1:CA:1321:U:C4    | 1:CA:1322:C:H5    | 2.36                     | 0.43              |
| 1:CA:135:C:O2     | 16:CP:1:MET:HB2   | 2.18                     | 0.43              |
| 1:CA:1361:G:H3'   | 1:CA:1362:A:C5'   | 2.47                     | 0.43              |
| 1:CA:1494:G:C6    | 1:CA:1495:U:C4    | 3.07                     | 0.43              |
| 1:CA:206:C:H2'    | 1:CA:207:C:C5'    | 2.46                     | 0.43              |
| 1:CA:32:A:N3      | 1:CA:33:A:C8      | 2.87                     | 0.43              |
| 1:CA:436:C:C2     | 1:CA:437:U:C5     | 3.06                     | 0.43              |
| 1:CA:57:G:C6      | 1:CA:58:C:C4      | 3.06                     | 0.43              |
| 1:CA:651:C:C4     | 1:CA:652:U:O4     | 2.72                     | 0.43              |
| 1:CA:847:G:C2     | 1:CA:848:C:C2     | 3.06                     | 0.43              |
| 1:CA:934:C:C5'    | 57:CA:1827:HOH:O  | 2.65                     | 0.43              |
| 4:CD:32:CYS:SG    | 4:CD:33:LYS:N     | 2.91                     | 0.43              |
| 8:CH:29:SER:HB2   | 8:CH:59:LEU:HB2   | 2.00                     | 0.43              |
| 8:CH:78:VAL:HG12  | 8:CH:79:SER:N     | 2.33                     | 0.43              |
| 12:CL:37:VAL:O    | 12:CL:37:VAL:HG12 | 2.18                     | 0.43              |
| 14:CN:87:ALA:HA   | 14:CN:92:GLU:HG3  | 2.00                     | 0.43              |
| 17:CQ:21:ILE:O    | 17:CQ:21:ILE:HG23 | 2.18                     | 0.43              |
| 17:CQ:75:LEU:C    | 17:CQ:75:LEU:CD1  | 2.87                     | 0.43              |
| 22:DA:1002:G:H2'  | 22:DA:1003:G:O5'  | 2.18                     | 0.43              |
| 22:DA:1176:U:N3   | 22:DA:1177:G:C6   | 2.86                     | 0.43              |
| 22:DA:1230:A:C6   | 22:DA:1231:U:N3   | 2.86                     | 0.43              |
| 22:DA:1257:C:C4   | 22:DA:1258:U:O4   | 2.71                     | 0.43              |
| 22:DA:1270:C:O2   | 22:DA:1325:U:O2'  | 2.36                     | 0.43              |
| 22:DA:1930:G:O2'  | 22:DA:1931:U:P    | 2.76                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:DA:1980:G:C2   | 22:DA:1982:U:C4   | 3.06                     | 0.43              |
| 22:DA:579:G:C5'   | 22:DA:2018:G:OP2  | 2.66                     | 0.43              |
| 22:DA:379:G:H4'   | 22:DA:2232:C:H5'' | 2.00                     | 0.43              |
| 22:DA:2264:C:C2   | 22:DA:2277:G:N2   | 2.86                     | 0.43              |
| 22:DA:2283:C:C2'  | 22:DA:2284:A:H5'  | 2.49                     | 0.43              |
| 22:DA:2311:A:H3'  | 22:DA:2312:U:C6   | 2.53                     | 0.43              |
| 22:DA:2370:G:C6   | 22:DA:2371:G:C6   | 3.07                     | 0.43              |
| 22:DA:2386:A:H2'  | 22:DA:2387:U:C6   | 2.53                     | 0.43              |
| 22:DA:2727:A:N1   | 22:DA:2728:U:C4   | 2.86                     | 0.43              |
| 22:DA:678:C:H2'   | 22:DA:679:C:C6    | 2.54                     | 0.43              |
| 25:DD:127:PHE:CE2 | 25:DD:160:LYS:HD2 | 2.53                     | 0.43              |
| 26:DE:24:ASN:O    | 26:DE:28:VAL:HG23 | 2.17                     | 0.43              |
| 22:DA:538:A:O2'   | 31:DJ:8:PRO:CG    | 2.65                     | 0.43              |
| 45:DX:47:VAL:O    | 45:DX:47:VAL:CG1  | 2.65                     | 0.43              |
| 47:DZ:24:LEU:HD11 | 47:DZ:54:MET:HE2  | 1.99                     | 0.43              |
| 1:AA:1319:A:C8    | 1:AA:1323:G:C6    | 3.06                     | 0.43              |
| 1:AA:1337:G:H5''  | 1:AA:1338:G:OP1   | 2.17                     | 0.43              |
| 1:AA:1369:C:H2'   | 1:AA:1370:G:C8    | 2.53                     | 0.43              |
| 1:AA:723:U:H5'    | 1:AA:724:G:P      | 2.59                     | 0.43              |
| 2:AB:24:ASN:HA    | 2:AB:25:PRO:HD2   | 1.78                     | 0.43              |
| 2:AB:79:ALA:O     | 2:AB:80:VAL:HG23  | 2.18                     | 0.43              |
| 4:AD:103:TYR:HB2  | 4:AD:114:ALA:HB2  | 2.00                     | 0.43              |
| 4:AD:121:LYS:HB3  | 4:AD:129:VAL:HG21 | 1.99                     | 0.43              |
| 4:AD:190:ASP:C    | 4:AD:191:LEU:HG   | 2.38                     | 0.43              |
| 6:AF:47:LEU:HD13  | 6:AF:51:ILE:HG23  | 1.99                     | 0.43              |
| 7:AG:145:ALA:C    | 7:AG:147:ALA:H    | 2.22                     | 0.43              |
| 7:AG:66:LEU:O     | 7:AG:70:ARG:HD3   | 2.18                     | 0.43              |
| 1:AA:641:U:H4'    | 8:AH:107:SER:O    | 2.18                     | 0.43              |
| 14:AN:15:ALA:O    | 14:AN:18:ASP:OD2  | 2.36                     | 0.43              |
| 16:AP:12:LYS:HG2  | 16:AP:13:LYS:HG2  | 2.00                     | 0.43              |
| 16:AP:8:ARG:HG3   | 16:AP:17:TYR:CE2  | 2.53                     | 0.43              |
| 19:AS:4:SER:HB2   | 19:AS:5:LEU:HD12  | 1.99                     | 0.43              |
| 20:AT:54:MET:CE   | 20:AT:58:VAL:HG21 | 2.48                     | 0.43              |
| 49:B1:34:LEU:HB3  | 49:B1:52:ALA:HB2  | 2.01                     | 0.43              |
| 53:B5:84:ILE:HG22 | 53:B5:84:ILE:O    | 2.18                     | 0.43              |
| 22:BA:1063:G:C6   | 22:BA:1064:C:H1'  | 2.54                     | 0.43              |
| 22:BA:1142:A:C2   | 22:BA:1144:A:N9   | 2.86                     | 0.43              |
| 22:BA:1168:G:N2   | 22:BA:1182:G:C4   | 2.86                     | 0.43              |
| 22:BA:1165:A:C2   | 22:BA:1185:G:C2   | 3.06                     | 0.43              |
| 22:BA:1193:G:O2'  | 22:BA:1194:A:H5'  | 2.18                     | 0.43              |
| 22:BA:1347:A:C2   | 22:BA:1348:C:H1'  | 2.53                     | 0.43              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 22:BA:1881:C:H2'   | 22:BA:1882:U:O4'  | 2.18                     | 0.43              |
| 22:BA:2001:C:C2    | 22:BA:2002:G:C8   | 3.06                     | 0.43              |
| 22:BA:2275:C:O2    | 34:BM:84:LYS:CD   | 2.66                     | 0.43              |
| 22:BA:255:A:H2'    | 22:BA:256:A:O4'   | 2.18                     | 0.43              |
| 22:BA:975:A:C8     | 22:BA:990:A:N6    | 2.86                     | 0.43              |
| 23:BB:99:A:H2'     | 23:BB:99:A:N3     | 2.33                     | 0.43              |
| 24:BC:209:GLY:O    | 24:BC:212:ARG:N   | 2.51                     | 0.43              |
| 25:BD:104:VAL:O    | 25:BD:105:LYS:CB  | 2.65                     | 0.43              |
| 26:BE:149:ILE:HD11 | 26:BE:172:ALA:CA  | 2.48                     | 0.43              |
| 29:BH:27:ARG:O     | 29:BH:28:ASN:CB   | 2.66                     | 0.43              |
| 29:BH:80:ILE:HG21  | 29:BH:94:ILE:HG13 | 2.00                     | 0.43              |
| 29:BH:96:THR:O     | 29:BH:100:ALA:N   | 2.50                     | 0.43              |
| 29:BH:9:VAL:O      | 29:BH:10:ALA:O    | 2.36                     | 0.43              |
| 30:BI:19:ASN:N     | 30:BI:20:PRO:HD2  | 2.33                     | 0.43              |
| 30:BI:42:PHE:O     | 30:BI:46:THR:OG1  | 2.32                     | 0.43              |
| 39:BR:79:ARG:O     | 39:BR:80:ARG:HB3  | 2.18                     | 0.43              |
| 40:BS:25:ARG:HB2   | 40:BS:74:ILE:CG2  | 2.49                     | 0.43              |
| 40:BS:74:ILE:HG23  | 40:BS:74:ILE:O    | 2.18                     | 0.43              |
| 41:BT:57:VAL:HG13  | 41:BT:86:THR:OG1  | 2.18                     | 0.43              |
| 43:BV:14:LYS:HD2   | 43:BV:18:ARG:NH1  | 2.33                     | 0.43              |
| 1:CA:1005:A:N7     | 1:CA:1006:G:C4    | 2.86                     | 0.43              |
| 1:CA:1018:G:O6     | 1:CA:1019:A:N6    | 2.51                     | 0.43              |
| 1:CA:1158:C:O2     | 1:CA:1158:C:C2'   | 2.66                     | 0.43              |
| 1:CA:1411:C:H2'    | 1:CA:1412:C:C6    | 2.53                     | 0.43              |
| 1:CA:1496:C:H2'    | 1:CA:1497:G:C1'   | 2.48                     | 0.43              |
| 1:CA:184:G:N2      | 1:CA:185:U:C2     | 2.87                     | 0.43              |
| 1:CA:420:U:O2'     | 1:CA:421:U:H5''   | 2.18                     | 0.43              |
| 1:CA:944:G:H5''    | 1:CA:945:G:OP2    | 2.18                     | 0.43              |
| 1:CA:946:A:H2'     | 1:CA:947:G:C8     | 2.53                     | 0.43              |
| 2:CB:206:ALA:O     | 2:CB:207:ILE:C    | 2.56                     | 0.43              |
| 5:CE:104:GLY:HA3   | 5:CE:122:ASN:O    | 2.18                     | 0.43              |
| 5:CE:12:GLN:HA     | 5:CE:12:GLN:OE1   | 2.17                     | 0.43              |
| 5:CE:133:PRO:HA    | 5:CE:136:VAL:HG13 | 2.00                     | 0.43              |
| 8:CH:95:VAL:O      | 8:CH:99:LEU:O     | 2.36                     | 0.43              |
| 20:CT:32:ILE:HG12  | 20:CT:54:MET:CE   | 2.47                     | 0.43              |
| 22:DA:1456:G:C6    | 22:DA:1457:U:C4   | 3.06                     | 0.43              |
| 22:DA:1905:C:O2'   | 22:DA:1929:G:H1'  | 2.18                     | 0.43              |
| 22:DA:2128:G:C6    | 22:DA:2129:C:C4   | 3.06                     | 0.43              |
| 22:DA:2116:G:C6    | 22:DA:2171:A:N6   | 2.86                     | 0.43              |
| 22:DA:2234:G:C5    | 22:DA:2235:G:N7   | 2.86                     | 0.43              |
| 22:DA:2467:C:H41   | 22:DA:2468:A:N6   | 2.16                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:DA:1783:A:H5'  | 22:DA:2608:G:H4'   | 1.99                     | 0.43              |
| 22:DA:2712:C:C2   | 22:DA:2715:C:OP1   | 2.71                     | 0.43              |
| 22:DA:2834:G:O6   | 22:DA:2879:A:C2'   | 2.65                     | 0.43              |
| 22:DA:520:G:H2'   | 22:DA:521:U:C6     | 2.54                     | 0.43              |
| 22:DA:53:A:C2     | 22:DA:179:C:H4'    | 2.52                     | 0.43              |
| 22:DA:590:A:H2'   | 22:DA:591:U:O4'    | 2.19                     | 0.43              |
| 22:DA:623:C:H2'   | 22:DA:624:C:O4'    | 2.19                     | 0.43              |
| 24:DC:251:GLN:HG2 | 24:DC:255:LYS:HB2  | 2.00                     | 0.43              |
| 26:DE:131:THR:HB  | 26:DE:164:LEU:HD22 | 1.99                     | 0.43              |
| 27:DF:123:ASP:N   | 27:DF:127:ASN:O    | 2.51                     | 0.43              |
| 37:DP:62:ARG:CZ   | 37:DP:101:ARG:HA   | 2.48                     | 0.43              |
| 38:DQ:27:ALA:HB1  | 38:DQ:31:VAL:CG2   | 2.48                     | 0.43              |
| 22:DA:1249:U:H4'  | 38:DQ:4:VAL:HB     | 1.99                     | 0.43              |
| 41:DT:20:ALA:HA   | 41:DT:31:VAL:HG21  | 2.00                     | 0.43              |
| 1:AA:1182:G:C4'   | 1:AA:1183:U:H5'    | 2.48                     | 0.43              |
| 1:AA:1251:A:H2'   | 1:AA:1252:A:O4'    | 2.18                     | 0.43              |
| 1:AA:1332:A:C8    | 1:AA:1333:A:C8     | 3.07                     | 0.43              |
| 1:AA:1415:G:C6    | 1:AA:1486:G:C6     | 3.07                     | 0.43              |
| 1:AA:174:A:C2'    | 1:AA:175:C:H5'     | 2.48                     | 0.43              |
| 1:AA:192:A:C2     | 1:AA:193:C:C2      | 3.06                     | 0.43              |
| 1:AA:32:A:C2      | 1:AA:33:A:C4       | 3.06                     | 0.43              |
| 1:AA:900:A:N1     | 1:AA:901:A:C2      | 2.87                     | 0.43              |
| 1:AA:947:G:C6     | 1:AA:948:C:C4      | 3.07                     | 0.43              |
| 1:AA:980:C:C5     | 1:AA:981:U:C4      | 3.06                     | 0.43              |
| 2:AB:115:LYS:NZ   | 2:AB:153:ASP:OD1   | 2.43                     | 0.43              |
| 5:AE:83:HIS:HB2   | 5:AE:84:PRO:CD     | 2.49                     | 0.43              |
| 6:AF:16:GLU:HG3   | 4:CD:188:ARG:HH12  | 1.82                     | 0.43              |
| 6:AF:14:GLN:OE1   | 6:AF:17:GLN:HB2    | 2.18                     | 0.43              |
| 6:AF:76:THR:O     | 6:AF:79:ARG:N      | 2.44                     | 0.43              |
| 9:AI:29:VAL:O     | 9:AI:30:ILE:HG22   | 2.18                     | 0.43              |
| 7:AG:16:PRO:HB2   | 9:AI:46:MET:HE3    | 2.00                     | 0.43              |
| 10:AJ:19:ASP:HA   | 10:AJ:22:THR:HB    | 2.00                     | 0.43              |
| 15:AO:24:SER:O    | 15:AO:25:THR:C     | 2.56                     | 0.43              |
| 17:AQ:41:THR:HG22 | 17:AQ:42:THR:N     | 2.33                     | 0.43              |
| 22:BA:1059:G:C5   | 22:BA:1080:A:C2    | 3.06                     | 0.43              |
| 22:BA:1059:G:C6   | 22:BA:1060:U:C4    | 3.07                     | 0.43              |
| 22:BA:1064:C:H2'  | 22:BA:1064:C:O2    | 2.17                     | 0.43              |
| 22:BA:1864:U:C5   | 22:BA:1865:U:C4    | 3.06                     | 0.43              |
| 22:BA:1941:C:C4   | 22:BA:1942:C:C4    | 3.05                     | 0.43              |
| 22:BA:226:A:N6    | 22:BA:227:A:C6     | 2.86                     | 0.43              |
| 22:BA:2694:G:H2'  | 22:BA:2695:U:H6    | 1.82                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:BA:315:G:H2'   | 22:BA:316:C:C6     | 2.53                     | 0.43              |
| 22:BA:999:U:C5    | 22:BA:1154:G:C6    | 3.06                     | 0.43              |
| 23:BB:29:A:H2'    | 23:BB:30:C:O4'     | 2.18                     | 0.43              |
| 24:BC:53:HIS:CD2  | 24:BC:219:THR:HA   | 2.54                     | 0.43              |
| 29:BH:76:GLU:HA   | 29:BH:142:VAL:HG12 | 2.00                     | 0.43              |
| 30:BI:28:LEU:HG   | 30:BI:35:ILE:CD1   | 2.48                     | 0.43              |
| 1:AA:346:G:P      | 32:BK:105:ARG:HH12 | 2.41                     | 0.43              |
| 32:BK:10:VAL:CG1  | 32:BK:12:ASP:OD1   | 2.67                     | 0.43              |
| 33:BL:81:ASP:CB   | 33:BL:100:ILE:HD12 | 2.48                     | 0.43              |
| 37:BP:103:ARG:HG3 | 37:BP:103:ARG:HH11 | 1.81                     | 0.43              |
| 38:BQ:76:TYR:CE2  | 38:BQ:80:ILE:HG13  | 2.53                     | 0.43              |
| 1:CA:1105:A:H2'   | 1:CA:1106:G:H8     | 1.83                     | 0.43              |
| 1:CA:1211:U:H1'   | 1:CA:1213:A:C2     | 2.53                     | 0.43              |
| 1:CA:195:A:C6     | 1:CA:196:A:N1      | 2.86                     | 0.43              |
| 1:CA:256:U:OP1    | 17:CQ:19:LYS:NZ    | 2.40                     | 0.43              |
| 1:CA:409:U:H5'    | 4:CD:25:VAL:HG23   | 2.00                     | 0.43              |
| 29:BH:91:PHE:HB3  | 1:CA:55:A:C4       | 2.54                     | 0.43              |
| 1:CA:718:A:OP2    | 1:CA:720:C:N4      | 2.50                     | 0.43              |
| 1:CA:583:A:C6     | 1:CA:759:A:N7      | 2.86                     | 0.43              |
| 1:CA:764:C:N4     | 1:CA:765:G:C5      | 2.87                     | 0.43              |
| 1:CA:919:A:N1     | 1:CA:920:U:C4      | 2.86                     | 0.43              |
| 1:CA:938:A:N6     | 1:CA:939:G:C5      | 2.86                     | 0.43              |
| 1:CA:983:A:H2'    | 1:CA:983:A:N3      | 2.33                     | 0.43              |
| 10:CJ:80:THR:O    | 10:CJ:84:VAL:HG12  | 2.18                     | 0.43              |
| 1:CA:718:A:H5'    | 11:CK:119:ASN:ND2  | 2.33                     | 0.43              |
| 16:CP:67:ILE:HG23 | 16:CP:71:VAL:CG1   | 2.49                     | 0.43              |
| 1:CA:1318:A:O2'   | 19:CS:37:ARG:HD2   | 2.19                     | 0.43              |
| 20:CT:36:TYR:CG   | 20:CT:37:ALA:N     | 2.87                     | 0.43              |
| 50:D2:43:THR:O    | 50:D2:44:VAL:CB    | 2.66                     | 0.43              |
| 22:DA:1364:G:C5   | 22:DA:1368:G:N1    | 2.87                     | 0.43              |
| 22:DA:1470:A:H2'  | 22:DA:1471:G:H5'   | 2.00                     | 0.43              |
| 22:DA:1486:U:N3   | 22:DA:1504:A:C2    | 2.86                     | 0.43              |
| 22:DA:1524:G:N3   | 22:DA:1525:A:C8    | 2.86                     | 0.43              |
| 22:DA:1595:C:H2'  | 22:DA:1596:A:O4'   | 2.19                     | 0.43              |
| 22:DA:1272:A:C2   | 22:DA:1618:A:C4    | 3.06                     | 0.43              |
| 22:DA:207:A:C2    | 22:DA:208:C:H1'    | 2.53                     | 0.43              |
| 22:DA:225:C:H2'   | 22:DA:226:A:O4'    | 2.18                     | 0.43              |
| 22:DA:305:C:C2    | 22:DA:313:G:N1     | 2.86                     | 0.43              |
| 22:DA:487:C:N4    | 22:DA:488:G:N1     | 2.67                     | 0.43              |
| 22:DA:599:A:H1'   | 22:DA:659:G:N2     | 2.34                     | 0.43              |
| 22:DA:647:G:C4    | 22:DA:648:G:C8     | 3.07                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:DA:64:A:H2'    | 22:DA:65:U:C6      | 2.53                     | 0.43              |
| 22:DA:679:C:H2'   | 22:DA:680:C:H6     | 1.82                     | 0.43              |
| 22:DA:717:C:N4    | 22:DA:718:A:N3     | 2.65                     | 0.43              |
| 22:DA:776:G:C8    | 22:DA:793:A:C5     | 3.07                     | 0.43              |
| 23:DB:114:C:O2'   | 23:DB:115:A:H5'    | 2.18                     | 0.43              |
| 23:DB:13:G:O2'    | 23:DB:15:A:H5'     | 2.18                     | 0.43              |
| 24:DC:64:ILE:O    | 24:DC:103:TYR:HB2  | 2.18                     | 0.43              |
| 25:DD:108:ASP:OD1 | 25:DD:207:VAL:HG12 | 2.18                     | 0.43              |
| 26:DE:130:LYS:CB  | 26:DE:133:LEU:HB2  | 2.48                     | 0.43              |
| 27:DF:9:LYS:O     | 27:DF:13:VAL:HG23  | 2.18                     | 0.43              |
| 27:DF:158:THR:OG1 | 27:DF:169:LEU:CD2  | 2.67                     | 0.43              |
| 28:DG:91:GLY:HA3  | 28:DG:160:LYS:HG3  | 2.00                     | 0.43              |
| 31:DJ:56:VAL:HB   | 31:DJ:124:VAL:HG12 | 2.00                     | 0.43              |
| 22:DA:538:A:O2'   | 31:DJ:8:PRO:HG3    | 2.18                     | 0.43              |
| 32:DK:7:MET:C     | 32:DK:8:LEU:HD12   | 2.38                     | 0.43              |
| 34:DM:78:LEU:O    | 34:DM:79:ALA:HB3   | 2.19                     | 0.43              |
| 37:DP:93:ARG:O    | 37:DP:94:LYS:HB2   | 2.18                     | 0.43              |
| 43:DV:42:LEU:HD12 | 43:DV:47:VAL:HG21  | 2.00                     | 0.43              |
| 45:DX:30:LEU:HB3  | 45:DX:31:PRO:CD    | 2.48                     | 0.43              |
| 45:DX:68:LEU:HD22 | 45:DX:78:TYR:CE1   | 2.53                     | 0.43              |
| 1:AA:1406:U:C6    | 1:AA:1407:C:C5     | 3.06                     | 0.43              |
| 1:AA:1529:G:H4'   | 1:AA:1530:G:OP2    | 2.18                     | 0.43              |
| 1:AA:567:G:N2     | 1:AA:568:G:H1'     | 2.33                     | 0.43              |
| 1:AA:77:A:H2'     | 1:AA:78:A:C8       | 2.53                     | 0.43              |
| 1:AA:780:A:C8     | 1:AA:800:G:O6      | 2.71                     | 0.43              |
| 1:AA:841:C:C2     | 1:AA:843:U:H5'     | 2.54                     | 0.43              |
| 1:AA:895:G:C6     | 1:AA:896:C:C4      | 3.06                     | 0.43              |
| 2:AB:106:THR:O    | 2:AB:107:VAL:CB    | 2.66                     | 0.43              |
| 3:AC:159:GLY:O    | 3:AC:160:ALA:C     | 2.57                     | 0.43              |
| 4:AD:145:ILE:N    | 4:AD:145:ILE:CD1   | 2.81                     | 0.43              |
| 4:AD:26:ARG:HD3   | 4:AD:31:LYS:HD2    | 2.01                     | 0.43              |
| 4:AD:88:GLU:O     | 4:AD:91:LEU:N      | 2.51                     | 0.43              |
| 9:AI:22:LYS:O     | 9:AI:62:ASP:HB2    | 2.18                     | 0.43              |
| 10:AJ:40:ILE:HB   | 10:AJ:73:LEU:HB2   | 2.00                     | 0.43              |
| 10:AJ:92:LEU:O    | 10:AJ:93:ALA:HB2   | 2.19                     | 0.43              |
| 17:AQ:17:MET:HB2  | 17:AQ:20:SER:HB3   | 2.01                     | 0.43              |
| 18:AR:52:GLN:HA   | 18:AR:52:GLN:OE1   | 2.17                     | 0.43              |
| 20:AT:54:MET:CE   | 20:AT:58:VAL:CG2   | 2.97                     | 0.43              |
| 21:AU:34:ARG:O    | 21:AU:36:GLU:N     | 2.52                     | 0.43              |
| 22:BA:1043:C:N4   | 22:BA:1044:C:N4    | 2.65                     | 0.43              |
| 22:BA:1189:A:H2'  | 22:BA:1190:G:O4'   | 2.18                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:BA:1404:C:N3   | 22:BA:1405:U:C5    | 2.86                     | 0.43              |
| 22:BA:141:G:N1    | 41:BT:1:MET:CE     | 2.82                     | 0.43              |
| 22:BA:2309:A:C6   | 22:BA:2310:C:C4    | 3.06                     | 0.43              |
| 22:BA:231:A:C6    | 22:BA:232:G:C2     | 3.07                     | 0.43              |
| 22:BA:2880:C:C2   | 22:BA:2881:U:C5    | 3.07                     | 0.43              |
| 22:BA:996:A:H4'   | 38:BQ:91:ASP:OD1   | 2.19                     | 0.43              |
| 24:BC:174:LEU:N   | 24:BC:174:LEU:CD1  | 2.82                     | 0.43              |
| 24:BC:77:VAL:HG22 | 24:BC:78:VAL:N     | 2.34                     | 0.43              |
| 25:BD:39:ASP:CG   | 25:BD:40:LEU:N     | 2.71                     | 0.43              |
| 26:BE:88:ARG:HB3  | 26:BE:89:PRO:HD2   | 2.01                     | 0.43              |
| 29:BH:41:LYS:HA   | 29:BH:44:ILE:HG12  | 2.01                     | 0.43              |
| 29:BH:94:ILE:CD1  | 29:BH:98:ASP:HB3   | 2.48                     | 0.43              |
| 30:BI:108:GLU:OE2 | 30:BI:109:ILE:CG1  | 2.67                     | 0.43              |
| 30:BI:67:PHE:N    | 30:BI:67:PHE:CD2   | 2.86                     | 0.43              |
| 31:BJ:93:ILE:CD1  | 31:BJ:100:VAL:HG21 | 2.49                     | 0.43              |
| 26:BE:32:VAL:HG21 | 33:BL:6:LEU:HD13   | 2.01                     | 0.43              |
| 36:BO:107:ALA:O   | 36:BO:111:ARG:HG3  | 2.17                     | 0.43              |
| 46:BY:54:LYS:HA   | 46:BY:57:LEU:HD23  | 2.00                     | 0.43              |
| 1:CA:1032:G:H2'   | 1:CA:1032:G:N3     | 2.34                     | 0.43              |
| 1:CA:1141:C:HO2'  | 1:CA:1142:G:C5'    | 2.30                     | 0.43              |
| 1:CA:1255:G:C6    | 1:CA:1279:G:C5     | 3.06                     | 0.43              |
| 1:CA:1424:U:H2'   | 1:CA:1425:U:O4'    | 2.17                     | 0.43              |
| 1:CA:1459:G:H2'   | 1:CA:1460:C:O4'    | 2.18                     | 0.43              |
| 1:CA:635:A:C5     | 1:CA:636:U:C4      | 3.07                     | 0.43              |
| 1:CA:678:U:H2'    | 1:CA:679:C:O4'     | 2.19                     | 0.43              |
| 1:CA:790:A:N6     | 1:CA:791:G:C6      | 2.87                     | 0.43              |
| 1:CA:947:G:N2     | 1:CA:1235:U:O2     | 2.52                     | 0.43              |
| 2:CB:141:LEU:O    | 2:CB:142:GLU:C     | 2.57                     | 0.43              |
| 2:CB:35:ARG:O     | 2:CB:38:VAL:HG12   | 2.18                     | 0.43              |
| 4:CD:192:SER:HB2  | 4:CD:195:ILE:HG12  | 2.01                     | 0.43              |
| 9:CI:24:GLY:N     | 9:CI:61:LEU:HA     | 2.34                     | 0.43              |
| 1:CA:1126:U:O4    | 10:CJ:73:LEU:CD1   | 2.66                     | 0.43              |
| 12:CL:74:LEU:HD11 | 12:CL:80:ILE:HG21  | 2.01                     | 0.43              |
| 16:CP:52:LEU:HD22 | 16:CP:57:ILE:HD11  | 2.01                     | 0.43              |
| 18:CR:25:ASP:C    | 18:CR:27:ALA:N     | 2.71                     | 0.43              |
| 20:CT:33:LYS:O    | 20:CT:36:TYR:CE2   | 2.71                     | 0.43              |
| 50:D2:31:LEU:CD2  | 50:D2:42:LEU:HB3   | 2.48                     | 0.43              |
| 22:DA:1203:U:O4   | 22:DA:1204:A:C6    | 2.72                     | 0.43              |
| 22:DA:1370:C:H2'  | 22:DA:1371:G:C8    | 2.54                     | 0.43              |
| 22:DA:1838:C:C6   | 22:DA:1899:A:C6    | 3.07                     | 0.43              |
| 22:DA:186:G:C2    | 22:DA:211:C:C2     | 3.06                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:DA:208:C:H2'    | 22:DA:209:C:C6     | 2.53                     | 0.43              |
| 22:DA:2415:G:C5    | 22:DA:2416:C:C5    | 3.07                     | 0.43              |
| 22:DA:830:G:C4     | 22:DA:2448:A:C5    | 3.06                     | 0.43              |
| 22:DA:2749:A:C8    | 22:DA:2750:A:H2'   | 2.52                     | 0.43              |
| 22:DA:2823:A:C5    | 22:DA:2824:C:C5    | 3.06                     | 0.43              |
| 22:DA:2720:U:C6    | 22:DA:2872:A:C6    | 3.07                     | 0.43              |
| 22:DA:605:G:C6     | 22:DA:606:U:C4     | 3.07                     | 0.43              |
| 22:DA:605:G:C5     | 22:DA:606:U:C5     | 3.07                     | 0.43              |
| 22:DA:616:A:H2'    | 22:DA:616:A:N3     | 2.33                     | 0.43              |
| 22:DA:661:A:H1'    | 33:DL:12:SER:O     | 2.17                     | 0.43              |
| 22:DA:870:U:OP1    | 34:DM:6:ARG:CD     | 2.66                     | 0.43              |
| 23:DB:71:C:C2      | 23:DB:106:G:N2     | 2.86                     | 0.43              |
| 23:DB:94:A:H2'     | 23:DB:95:U:O4'     | 2.18                     | 0.43              |
| 24:DC:69:ARG:NH2   | 24:DC:116:ILE:HD11 | 2.33                     | 0.43              |
| 24:DC:147:LYS:HB2  | 24:DC:150:LYS:CB   | 2.49                     | 0.43              |
| 24:DC:221:ARG:NH2  | 57:DC:306:HOH:O    | 2.51                     | 0.43              |
| 25:DD:167:ASN:O    | 25:DD:168:GLU:HB3  | 2.18                     | 0.43              |
| 25:DD:193:VAL:HB   | 25:DD:194:PRO:CD   | 2.49                     | 0.43              |
| 27:DF:40:VAL:HG13  | 27:DF:41:GLY:N     | 2.34                     | 0.43              |
| 30:DI:67:PHE:CD2   | 30:DI:67:PHE:N     | 2.86                     | 0.43              |
| 32:DK:92:GLU:N     | 32:DK:92:GLU:OE2   | 2.49                     | 0.43              |
| 37:DP:100:LEU:HD22 | 37:DP:108:ALA:HB1  | 2.00                     | 0.43              |
| 22:DA:1248:G:C5    | 38:DQ:3:ARG:HB2    | 2.53                     | 0.43              |
| 40:DS:33:LEU:CD2   | 40:DS:52:GLU:HG3   | 2.48                     | 0.43              |
| 1:AA:1109:C:P      | 3:AC:176:HIS:CE1   | 3.12                     | 0.43              |
| 1:AA:1158:C:N3     | 1:AA:1160:G:N7     | 2.67                     | 0.43              |
| 1:AA:1176:A:H3'    | 1:AA:1177:G:C8     | 2.54                     | 0.43              |
| 1:AA:130:A:N1      | 1:AA:233:C:O2'     | 2.42                     | 0.43              |
| 1:AA:39:G:N3       | 1:AA:40:C:C6       | 2.87                     | 0.43              |
| 1:AA:457:G:H5'     | 1:AA:458:U:OP2     | 2.18                     | 0.43              |
| 1:AA:474:G:C5      | 1:AA:475:C:C5      | 3.06                     | 0.43              |
| 1:AA:692:U:O2      | 1:AA:694:A:C8      | 2.70                     | 0.43              |
| 1:AA:810:C:H2'     | 1:AA:810:C:O2      | 2.18                     | 0.43              |
| 1:AA:849:G:C5      | 1:AA:850:U:C4      | 3.06                     | 0.43              |
| 1:AA:927:G:N1      | 1:AA:1391:U:C2     | 2.86                     | 0.43              |
| 2:AB:119:THR:O     | 2:AB:120:GLN:HB2   | 2.18                     | 0.43              |
| 2:AB:83:ALA:O      | 2:AB:86:SER:OG     | 2.35                     | 0.43              |
| 3:AC:203:PHE:CE1   | 3:AC:205:GLY:O     | 2.72                     | 0.43              |
| 4:AD:161:LEU:HD22  | 4:AD:161:LEU:N     | 2.34                     | 0.43              |
| 4:AD:3:ARG:NH2     | 4:AD:115:ARG:HD3   | 2.33                     | 0.43              |
| 5:AE:156:LYS:HB3   | 8:AH:71:VAL:HG13   | 2.01                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AA:1081:A:H5'   | 5:AE:23:LYS:HG3   | 2.01                     | 0.43              |
| 8:AH:21:ASN:HA    | 8:AH:65:TYR:CE1   | 2.53                     | 0.43              |
| 9:AI:30:ILE:O     | 9:AI:33:ARG:N     | 2.52                     | 0.43              |
| 12:AL:38:TYR:O    | 12:AL:39:THR:HG22 | 2.18                     | 0.43              |
| 49:B1:29:THR:C    | 49:B1:31:PRO:CD   | 2.85                     | 0.43              |
| 22:BA:1086:A:O2'  | 22:BA:1087:G:N7   | 2.49                     | 0.43              |
| 22:BA:1496:A:N3   | 22:BA:1577:C:O2'  | 2.46                     | 0.43              |
| 22:BA:1607:C:N4   | 22:BA:1622:G:C5   | 2.86                     | 0.43              |
| 22:BA:1712:U:C4   | 22:BA:1713:A:C5   | 3.07                     | 0.43              |
| 22:BA:1867:G:C2'  | 22:BA:1868:C:H5'  | 2.49                     | 0.43              |
| 22:BA:1923:U:H2'  | 22:BA:1923:U:O2   | 2.17                     | 0.43              |
| 22:BA:191:A:H2'   | 22:BA:192:C:C6    | 2.53                     | 0.43              |
| 22:BA:2078:C:O2'  | 22:BA:2079:U:H5'  | 2.18                     | 0.43              |
| 22:BA:2117:A:N1   | 22:BA:2170:A:N1   | 2.66                     | 0.43              |
| 22:BA:2190:G:N2   | 22:BA:2191:A:H1'  | 2.33                     | 0.43              |
| 22:BA:2360:G:H4'  | 33:BL:61:LEU:HD21 | 2.00                     | 0.43              |
| 22:BA:417:C:H2'   | 22:BA:418:C:H6    | 1.82                     | 0.43              |
| 22:BA:773:U:O2'   | 24:BC:48:ARG:HD3  | 2.19                     | 0.43              |
| 24:BC:30:PHE:CZ   | 24:BC:32:PRO:HG2  | 2.53                     | 0.43              |
| 25:BD:13:ARG:HD3  | 25:BD:21:SER:OG   | 2.19                     | 0.43              |
| 26:BE:59:PRO:HD3  | 26:BE:71:GLY:O    | 2.19                     | 0.43              |
| 27:BF:158:THR:CG2 | 27:BF:160:ALA:HB3 | 2.48                     | 0.43              |
| 27:BF:64:LYS:HA   | 27:BF:65:PRO:HD3  | 1.90                     | 0.43              |
| 28:BG:38:ASN:O    | 28:BG:39:ASP:HB2  | 2.19                     | 0.43              |
| 29:BH:103:VAL:O   | 29:BH:108:VAL:O   | 2.37                     | 0.43              |
| 33:BL:68:SER:HB3  | 33:BL:71:ALA:CB   | 2.49                     | 0.43              |
| 33:BL:81:ASP:O    | 33:BL:82:LEU:HB3  | 2.18                     | 0.43              |
| 33:BL:82:LEU:C    | 33:BL:82:LEU:HD23 | 2.38                     | 0.43              |
| 23:BB:90:C:H5'    | 34:BM:18:ARG:HG3  | 2.00                     | 0.43              |
| 41:BT:29:THR:OG1  | 41:BT:86:THR:HG22 | 2.19                     | 0.43              |
| 41:BT:89:GLU:O    | 41:BT:91:GLN:N    | 2.52                     | 0.43              |
| 42:BU:54:GLN:N    | 42:BU:55:PRO:CD   | 2.81                     | 0.43              |
| 45:BX:74:ARG:NH2  | 45:BX:76:GLU:HG3  | 2.33                     | 0.43              |
| 1:CA:104:G:C2     | 1:CA:105:G:C8     | 3.06                     | 0.43              |
| 1:CA:129:A:H1'    | 1:CA:130:A:C8     | 2.54                     | 0.43              |
| 1:CA:1316:G:N2    | 1:CA:1318:A:H3'   | 2.33                     | 0.43              |
| 1:CA:1306:A:H1'   | 1:CA:1332:A:N7    | 2.34                     | 0.43              |
| 1:CA:1323:G:O2'   | 1:CA:1362:A:N3    | 2.40                     | 0.43              |
| 1:CA:258:G:H2'    | 1:CA:259:G:O4'    | 2.18                     | 0.43              |
| 1:CA:38:G:N2      | 1:CA:397:A:C4     | 2.86                     | 0.43              |
| 1:CA:216:U:C5'    | 1:CA:464:U:H4'    | 2.47                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 1:CA:632:U:H5''   | 1:CA:633:G:C8      | 2.54                     | 0.43              |
| 1:CA:671:G:C6     | 1:CA:672:U:N3      | 2.86                     | 0.43              |
| 1:CA:794:A:H2'    | 1:CA:795:C:C6      | 2.52                     | 0.43              |
| 2:CB:68:LEU:HG    | 2:CB:154:MET:HE1   | 2.01                     | 0.43              |
| 2:CB:87:CYS:SG    | 2:CB:89:GLN:OE1    | 2.76                     | 0.43              |
| 4:CD:138:SER:HB3  | 4:CD:139:PRO:CD    | 2.48                     | 0.43              |
| 5:CE:133:PRO:HG2  | 5:CE:134:ILE:HD12  | 2.00                     | 0.43              |
| 7:CG:42:ILE:CG2   | 7:CG:116:MET:HG3   | 2.49                     | 0.43              |
| 7:CG:95:ARG:O     | 7:CG:99:LEU:HG     | 2.19                     | 0.43              |
| 10:CJ:8:ILE:CD1   | 10:CJ:25:ILE:HD11  | 2.48                     | 0.43              |
| 22:DA:1208:C:N4   | 22:DA:1209:U:O4    | 2.52                     | 0.43              |
| 22:DA:1365:A:H3'  | 22:DA:1366:A:C8    | 2.54                     | 0.43              |
| 22:DA:1439:A:C2   | 22:DA:1553:A:C4    | 3.06                     | 0.43              |
| 22:DA:1594:U:H2'  | 22:DA:1595:C:C6    | 2.53                     | 0.43              |
| 22:DA:1802:A:N1   | 22:DA:1803:A:C2    | 2.86                     | 0.43              |
| 22:DA:1803:A:N1   | 22:DA:1822:C:O2'   | 2.49                     | 0.43              |
| 22:DA:1851:U:H2'  | 22:DA:1852:U:O4'   | 2.19                     | 0.43              |
| 22:DA:1989:G:H2'  | 22:DA:1990:C:H5'   | 2.00                     | 0.43              |
| 22:DA:2057:G:H2'  | 22:DA:2058:A:O4'   | 2.19                     | 0.43              |
| 22:DA:2201:G:C4   | 22:DA:2202:U:C5    | 3.06                     | 0.43              |
| 22:DA:2335:A:N6   | 22:DA:2337:G:H1'   | 2.34                     | 0.43              |
| 22:DA:2409:G:H2'  | 22:DA:2410:G:O4'   | 2.17                     | 0.43              |
| 22:DA:2547:A:C8   | 22:DA:2566:A:C8    | 3.06                     | 0.43              |
| 22:DA:485:C:C2    | 22:DA:496:G:C2     | 3.07                     | 0.43              |
| 22:DA:586:A:C8    | 22:DA:586:A:OP2    | 2.72                     | 0.43              |
| 22:DA:621:A:OP2   | 33:DL:99:ASN:ND2   | 2.51                     | 0.43              |
| 23:DB:34:A:N6     | 23:DB:44:G:H1'     | 2.33                     | 0.43              |
| 22:DA:1829:A:HO2' | 24:DC:15:HIS:CD2   | 2.36                     | 0.43              |
| 24:DC:183:LYS:O   | 24:DC:184:VAL:HG23 | 2.18                     | 0.43              |
| 25:DD:28:GLU:HA   | 25:DD:185:ASN:O    | 2.19                     | 0.43              |
| 26:DE:170:ARG:NH1 | 26:DE:176:ASP:OD1  | 2.52                     | 0.43              |
| 22:DA:443:A:C8    | 26:DE:40:ARG:HD3   | 2.54                     | 0.43              |
| 27:DF:31:VAL:O    | 27:DF:31:VAL:HG13  | 2.19                     | 0.43              |
| 28:DG:91:GLY:O    | 28:DG:94:TYR:CD1   | 2.72                     | 0.43              |
| 31:DJ:106:LYS:HD2 | 31:DJ:119:PHE:CZ   | 2.54                     | 0.43              |
| 32:DK:10:VAL:HB   | 32:DK:16:ALA:O     | 2.19                     | 0.43              |
| 22:DA:1277:G:H5'  | 35:DN:20:MET:HE1   | 1.99                     | 0.43              |
| 36:DO:49:VAL:HG12 | 36:DO:50:ALA:N     | 2.33                     | 0.43              |
| 37:DP:79:PRO:O    | 37:DP:80:VAL:C     | 2.57                     | 0.43              |
| 39:DR:68:ARG:HD3  | 39:DR:92:TRP:CE2   | 2.54                     | 0.43              |
| 41:DT:67:VAL:CG1  | 41:DT:68:LYS:N     | 2.80                     | 0.43              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 42:DU:3:ALA:O      | 42:DU:6:ARG:NH1   | 2.52                     | 0.43              |
| 47:DZ:13:ALA:HB2   | 47:DZ:24:LEU:HD12 | 1.99                     | 0.43              |
| 1:AA:1173:U:H2'    | 1:AA:1174:G:C8    | 2.54                     | 0.43              |
| 1:AA:1492:A:OP1    | 12:AL:44:LYS:CA   | 2.66                     | 0.43              |
| 1:AA:202:G:O2'     | 1:AA:468:A:C8     | 2.67                     | 0.43              |
| 1:AA:607:A:C6      | 1:AA:608:A:C6     | 3.06                     | 0.43              |
| 1:AA:686:U:O4      | 1:AA:703:G:O2'    | 2.30                     | 0.43              |
| 1:AA:895:G:C5      | 1:AA:896:C:C5     | 3.07                     | 0.43              |
| 1:AA:949:A:C2'     | 1:AA:950:U:H5'    | 2.48                     | 0.43              |
| 1:AA:986:U:C2      | 1:AA:987:G:C8     | 3.07                     | 0.43              |
| 2:AB:57:LEU:HD11   | 2:AB:221:VAL:CG2  | 2.49                     | 0.43              |
| 9:AI:6:TYR:CB      | 9:AI:89:GLU:OE2   | 2.67                     | 0.43              |
| 10:AJ:65:TYR:HH    | 14:AN:85:ARG:HD2  | 1.83                     | 0.43              |
| 14:AN:84:VAL:HG12  | 14:AN:85:ARG:N    | 2.33                     | 0.43              |
| 15:AO:87:LEU:CD2   | 15:AO:87:LEU:N    | 2.81                     | 0.43              |
| 1:AA:264:C:O2'     | 17:AQ:66:PRO:O    | 2.25                     | 0.43              |
| 19:AS:40:ILE:HG13  | 19:AS:71:LEU:HD22 | 2.00                     | 0.43              |
| 49:B1:17:THR:CG2   | 49:B1:43:VAL:HG13 | 2.48                     | 0.43              |
| 49:B1:23:THR:OG1   | 49:B1:24:THR:N    | 2.51                     | 0.43              |
| 22:BA:1075:C:H2'   | 22:BA:1076:C:N1   | 2.34                     | 0.43              |
| 22:BA:1469:A:H2'   | 22:BA:1470:A:C8   | 2.54                     | 0.43              |
| 22:BA:1499:C:C4    | 22:BA:1500:G:N7   | 2.87                     | 0.43              |
| 22:BA:1587:G:C5    | 22:BA:1588:G:N7   | 2.87                     | 0.43              |
| 22:BA:2006:C:O2'   | 22:BA:2823:A:O2'  | 2.21                     | 0.43              |
| 22:BA:2201:G:C4    | 22:BA:2223:G:N2   | 2.87                     | 0.43              |
| 22:BA:2555:U:H5''  | 22:BA:2556:C:OP2  | 2.19                     | 0.43              |
| 22:BA:2598:A:N7    | 22:BA:2599:G:H1'  | 2.34                     | 0.43              |
| 22:BA:2607:G:H2'   | 22:BA:2608:G:O4'  | 2.17                     | 0.43              |
| 22:BA:2847:U:C2'   | 22:BA:2848:G:H5'  | 2.49                     | 0.43              |
| 22:BA:820:A:H2'    | 22:BA:821:A:O4'   | 2.17                     | 0.43              |
| 23:BB:22:U:H2'     | 23:BB:23:G:C8     | 2.54                     | 0.43              |
| 24:BC:76:ALA:HB2   | 24:BC:96:TYR:CG   | 2.54                     | 0.43              |
| 27:BF:158:THR:HG22 | 27:BF:160:ALA:H   | 1.83                     | 0.43              |
| 22:BA:832:U:H5'    | 33:BL:38:GLN:OE1  | 2.19                     | 0.43              |
| 36:BO:12:THR:O     | 36:BO:16:ARG:HG3  | 2.19                     | 0.43              |
| 40:BS:42:LYS:O     | 40:BS:42:LYS:HG2  | 2.18                     | 0.43              |
| 41:BT:47:VAL:HG12  | 41:BT:55:VAL:CG2  | 2.48                     | 0.43              |
| 43:BV:40:ILE:HG21  | 43:BV:42:LEU:HD21 | 1.99                     | 0.43              |
| 43:BV:83:LYS:O     | 43:BV:85:LYS:N    | 2.52                     | 0.43              |
| 46:BY:49:ASP:O     | 46:BY:52:ARG:HB2  | 2.19                     | 0.43              |
| 1:CA:1006:G:OP1    | 1:CA:1038:C:C5'   | 2.66                     | 0.43              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:110:C:N4      | 1:CA:111:G:C6      | 2.86                     | 0.43              |
| 1:CA:1151:A:C2     | 1:CA:1152:A:C4     | 3.07                     | 0.43              |
| 1:CA:1359:C:H2'    | 1:CA:1361:G:OP2    | 2.18                     | 0.43              |
| 1:CA:924:C:O2'     | 1:CA:1502:A:N1     | 2.44                     | 0.43              |
| 1:CA:68:G:O4'      | 1:CA:171:A:H1'     | 2.19                     | 0.43              |
| 1:CA:322:C:O2      | 1:CA:332:G:N2      | 2.43                     | 0.43              |
| 1:CA:538:G:H2'     | 1:CA:539:A:O4'     | 2.18                     | 0.43              |
| 1:CA:963:G:C2      | 1:CA:973:G:C6      | 3.06                     | 0.43              |
| 2:CB:16:PHE:CE1    | 2:CB:18:HIS:CE1    | 3.06                     | 0.43              |
| 3:CC:111:LEU:CD2   | 3:CC:111:LEU:N     | 2.82                     | 0.43              |
| 3:CC:34:ASP:CG     | 14:CN:65:ARG:HG2   | 2.39                     | 0.43              |
| 6:CF:52:ASN:O      | 6:CF:53:LYS:HB2    | 2.19                     | 0.43              |
| 1:CA:643:C:C5'     | 8:CH:32:LEU:CD2    | 2.97                     | 0.43              |
| 9:CI:25:ASN:O      | 9:CI:27:LYS:HG2    | 2.18                     | 0.43              |
| 11:CK:18:ASP:CB    | 11:CK:81:ASN:OD1   | 2.66                     | 0.43              |
| 12:CL:14:ARG:NH1   | 12:CL:15:LYS:HG3   | 2.33                     | 0.43              |
| 21:CU:39:GLU:HA    | 21:CU:42:THR:OG1   | 2.19                     | 0.43              |
| 50:D2:34:ARG:HD3   | 50:D2:42:LEU:O     | 2.18                     | 0.43              |
| 22:DA:1060:U:OP2   | 30:DI:75:PRO:HA    | 2.18                     | 0.43              |
| 22:DA:1356:G:C2    | 22:DA:1376:C:O2    | 2.72                     | 0.43              |
| 22:DA:1671:U:O2'   | 22:DA:1673:G:N7    | 2.35                     | 0.43              |
| 22:DA:1717:A:H2'   | 22:DA:1718:G:O4'   | 2.19                     | 0.43              |
| 22:DA:1805:A:N3    | 22:DA:1813:G:N2    | 2.66                     | 0.43              |
| 22:DA:2320:U:H5'   | 22:DA:2321:U:C5    | 2.53                     | 0.43              |
| 22:DA:2408:U:H2'   | 22:DA:2409:G:C8    | 2.54                     | 0.43              |
| 22:DA:2683:C:OP1   | 37:DP:56:HIS:HB3   | 2.18                     | 0.43              |
| 22:DA:2815:C:HO2'  | 48:D0:41:HIS:CE1   | 2.36                     | 0.43              |
| 22:DA:108:G:H1'    | 22:DA:347:A:N3     | 2.33                     | 0.43              |
| 22:DA:41:C:O2      | 22:DA:438:G:N2     | 2.48                     | 0.43              |
| 22:DA:55:G:H2'     | 22:DA:55:G:N3      | 2.34                     | 0.43              |
| 22:DA:668:A:C2     | 22:DA:670:A:C6     | 3.07                     | 0.43              |
| 22:DA:772:C:C2     | 22:DA:773:U:C6     | 3.07                     | 0.43              |
| 22:DA:828:U:H2'    | 22:DA:829:A:C8     | 2.54                     | 0.43              |
| 22:DA:963:U:H2'    | 22:DA:964:C:C6     | 2.53                     | 0.43              |
| 24:DC:126:PRO:HA   | 24:DC:192:LEU:O    | 2.19                     | 0.43              |
| 24:DC:67:PHE:CE2   | 24:DC:156:ARG:CZ   | 3.02                     | 0.43              |
| 24:DC:141:VAL:HG13 | 24:DC:191:THR:O    | 2.18                     | 0.43              |
| 27:DF:29:PRO:CB    | 27:DF:169:LEU:HD22 | 2.49                     | 0.43              |
| 22:DA:1063:G:O4'   | 30:DI:77:ALA:HB1   | 2.17                     | 0.43              |
| 30:DI:8:TYR:CB     | 30:DI:59:ILE:H     | 2.32                     | 0.43              |
| 31:DJ:114:LEU:O    | 31:DJ:118:MET:HG2  | 2.18                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 43:DV:41:GLU:C    | 43:DV:42:LEU:HD23  | 2.39                     | 0.43              |
| 1:AA:1501:C:C4    | 1:AA:1504:G:C5     | 3.07                     | 0.43              |
| 1:AA:41:G:H2'     | 1:AA:42:G:C8       | 2.54                     | 0.43              |
| 1:AA:482:A:H2'    | 1:AA:483:C:O4'     | 2.19                     | 0.43              |
| 1:AA:704:A:N6     | 1:AA:705:G:C6      | 2.86                     | 0.43              |
| 1:AA:946:A:C6     | 1:AA:947:G:C6      | 3.06                     | 0.43              |
| 5:AE:74:VAL:HG23  | 5:AE:76:LEU:HD12   | 1.99                     | 0.43              |
| 7:AG:67:GLU:HA    | 7:AG:70:ARG:HE     | 1.84                     | 0.43              |
| 8:AH:78:VAL:HG21  | 8:AH:128:TYR:CD1   | 2.53                     | 0.43              |
| 12:AL:5:ASN:HB3   | 12:AL:9:ARG:NH1    | 2.34                     | 0.43              |
| 16:AP:67:ILE:CG2  | 16:AP:71:VAL:HG12  | 2.49                     | 0.43              |
| 1:AA:1014:A:C2    | 19:AS:34:TRP:CE2   | 3.07                     | 0.43              |
| 19:AS:58:VAL:CG1  | 19:AS:75:ALA:CB    | 2.97                     | 0.43              |
| 20:AT:9:LYS:O     | 20:AT:12:ILE:HG12  | 2.19                     | 0.43              |
| 22:BA:1115:G:C2   | 22:BA:1116:G:C5    | 3.07                     | 0.43              |
| 22:BA:1467:U:C5   | 22:BA:1546:G:N3    | 2.87                     | 0.43              |
| 22:BA:1603:A:H5'' | 57:BA:3414:HOH:O   | 2.18                     | 0.43              |
| 22:BA:1717:A:C2   | 22:BA:1718:G:H1'   | 2.54                     | 0.43              |
| 22:BA:1731:G:C4   | 22:BA:1733:G:C8    | 3.07                     | 0.43              |
| 22:BA:2190:G:C6   | 22:BA:2191:A:C4    | 3.06                     | 0.43              |
| 22:BA:2633:G:H2'  | 22:BA:2634:A:O4'   | 2.19                     | 0.43              |
| 22:BA:2650:U:C2'  | 22:BA:2651:C:H5'   | 2.49                     | 0.43              |
| 22:BA:528:A:C2    | 22:BA:2043:C:C5'   | 2.97                     | 0.43              |
| 22:BA:829:A:N7    | 22:BA:2247:A:O2'   | 2.49                     | 0.43              |
| 22:BA:912:C:C2'   | 22:BA:913:U:H5'    | 2.48                     | 0.43              |
| 23:BB:91:C:H2'    | 23:BB:92:C:H6      | 1.84                     | 0.43              |
| 24:BC:157:SER:O   | 24:BC:158:ALA:C    | 2.56                     | 0.43              |
| 29:BH:45:GLU:HA   | 29:BH:48:GLU:HB2   | 2.01                     | 0.43              |
| 30:BI:99:GLY:C    | 30:BI:100:LYS:HG2  | 2.39                     | 0.43              |
| 30:BI:103:ARG:HE  | 30:BI:104:ALA:N    | 2.17                     | 0.43              |
| 22:BA:538:A:H4'   | 31:BJ:7:LYS:HG2    | 2.01                     | 0.43              |
| 22:BA:1250:G:OP2  | 33:BL:21:ARG:NH2   | 2.52                     | 0.43              |
| 34:BM:57:VAL:O    | 34:BM:58:LYS:HG3   | 2.19                     | 0.43              |
| 40:BS:69:LEU:HG   | 40:BS:107:VAL:HG22 | 2.01                     | 0.43              |
| 1:CA:1124:G:C2'   | 1:CA:1145:A:H62    | 2.32                     | 0.43              |
| 1:CA:1375:A:C5    | 1:CA:1376:U:C5     | 3.06                     | 0.43              |
| 1:CA:1412:C:O2    | 1:CA:1413:A:C8     | 2.72                     | 0.43              |
| 1:CA:280:C:H4'    | 1:CA:281:G:OP2     | 2.19                     | 0.43              |
| 1:CA:32:A:C2      | 1:CA:33:A:N7       | 2.86                     | 0.43              |
| 1:CA:794:A:C5     | 1:CA:795:C:C4      | 3.06                     | 0.43              |
| 1:CA:860:A:N6     | 1:CA:861:G:C2      | 2.86                     | 0.43              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:CA:996:A:H2'     | 1:CA:997:U:C5     | 2.54                     | 0.43              |
| 3:CC:22:TRP:CH2    | 14:CN:94:PRO:HG2  | 2.53                     | 0.43              |
| 7:CG:49:THR:O      | 7:CG:53:ARG:HD3   | 2.18                     | 0.43              |
| 14:CN:54:ASP:OD1   | 14:CN:59:ARG:NH1  | 2.52                     | 0.43              |
| 17:CQ:14:SER:HB3   | 17:CQ:22:VAL:HG12 | 2.01                     | 0.43              |
| 19:CS:16:LEU:O     | 19:CS:20:GLU:HG2  | 2.17                     | 0.43              |
| 22:DA:1207:C:O2    | 22:DA:1239:G:N2   | 2.42                     | 0.43              |
| 22:DA:1219:U:H2'   | 22:DA:1220:G:C8   | 2.54                     | 0.43              |
| 22:DA:149:A:C2'    | 22:DA:150:U:H5'   | 2.49                     | 0.43              |
| 22:DA:1668:A:H4'   | 22:DA:1669:A:O5'  | 2.18                     | 0.43              |
| 22:DA:1670:C:C5    | 22:DA:1671:U:C4   | 3.07                     | 0.43              |
| 22:DA:1722:A:C6    | 22:DA:1739:A:C8   | 3.06                     | 0.43              |
| 22:DA:2185:U:H2'   | 22:DA:2186:G:C8   | 2.54                     | 0.43              |
| 22:DA:2282:G:H1'   | 22:DA:2390:U:C4   | 2.54                     | 0.43              |
| 22:DA:2350:C:H2'   | 22:DA:2351:G:O4'  | 2.18                     | 0.43              |
| 22:DA:2418:A:OP1   | 51:D3:45:ARG:NH1  | 2.52                     | 0.43              |
| 22:DA:2786:U:H2'   | 22:DA:2787:C:C6   | 2.54                     | 0.43              |
| 22:DA:2868:A:C6    | 22:DA:2869:G:C6   | 3.06                     | 0.43              |
| 22:DA:2898:U:H2'   | 22:DA:2899:A:C8   | 2.54                     | 0.43              |
| 22:DA:565:C:H2'    | 22:DA:566:U:O4'   | 2.19                     | 0.43              |
| 22:DA:618:G:C6     | 22:DA:619:G:C4    | 3.07                     | 0.43              |
| 22:DA:632:A:H4'    | 33:DL:68:SER:HB2  | 2.00                     | 0.43              |
| 22:DA:77:G:C2      | 22:DA:78:U:C2     | 3.06                     | 0.43              |
| 22:DA:819:A:C8     | 22:DA:1188:U:O4   | 2.71                     | 0.43              |
| 24:DC:226:ASN:HB3  | 24:DC:227:PRO:CD  | 2.49                     | 0.43              |
| 25:DD:178:VAL:HG12 | 25:DD:179:ARG:HG3 | 2.01                     | 0.43              |
| 26:DE:52:VAL:HG21  | 26:DE:81:GLY:CA   | 2.48                     | 0.43              |
| 27:DF:161:LYS:HB2  | 27:DF:165:GLU:OE1 | 2.19                     | 0.43              |
| 29:DH:62:LEU:HD13  | 29:DH:63:ALA:N    | 2.34                     | 0.43              |
| 39:DR:27:ILE:HG13  | 39:DR:33:VAL:HG11 | 2.01                     | 0.43              |
| 22:DA:566:U:C5     | 39:DR:80:ARG:HD3  | 2.54                     | 0.43              |
| 41:DT:11:LEU:CD2   | 41:DT:34:VAL:HG12 | 2.49                     | 0.43              |
| 1:AA:1049:U:H4'    | 1:AA:1050:G:OP2   | 2.18                     | 0.43              |
| 1:AA:1202:U:N3     | 1:AA:1203:C:C6    | 2.86                     | 0.43              |
| 1:AA:960:U:O2'     | 1:AA:1223:C:C5'   | 2.67                     | 0.43              |
| 1:AA:1269:A:H2     | 1:AA:1312:G:N3    | 2.16                     | 0.43              |
| 1:AA:1326:U:H2'    | 1:AA:1327:C:C6    | 2.54                     | 0.43              |
| 1:AA:1405:G:H1'    | 1:AA:1519:A:O4'   | 2.18                     | 0.43              |
| 1:AA:425:G:H2'     | 1:AA:426:U:O4'    | 2.19                     | 0.43              |
| 1:AA:539:A:N6      | 1:AA:540:G:O6     | 2.52                     | 0.43              |
| 1:AA:722:G:C2'     | 1:AA:723:U:OP2    | 2.67                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AA:946:A:H2'    | 1:AA:947:G:C8     | 2.54                     | 0.43              |
| 2:AB:164:ILE:HD12 | 2:AB:210:VAL:CG1  | 2.49                     | 0.43              |
| 2:AB:50:PHE:CE2   | 2:AB:51:ASN:OD1   | 2.72                     | 0.43              |
| 4:AD:26:ARG:NH1   | 4:AD:31:LYS:HB3   | 2.34                     | 0.43              |
| 9:AI:84:THR:HG21  | 9:AI:103:PHE:HB2  | 2.00                     | 0.43              |
| 11:AK:23:ILE:HD12 | 11:AK:23:ILE:C    | 2.39                     | 0.43              |
| 12:AL:107:VAL:CG2 | 12:AL:117:TYR:HB3 | 2.48                     | 0.43              |
| 17:AQ:9:GLN:HA    | 17:AQ:59:VAL:O    | 2.19                     | 0.43              |
| 19:AS:23:VAL:HG12 | 19:AS:24:GLU:N    | 2.34                     | 0.43              |
| 22:BA:1098:A:N7   | 22:BA:1099:G:C6   | 2.86                     | 0.43              |
| 22:BA:996:A:C6    | 22:BA:1160:G:C2   | 3.07                     | 0.43              |
| 22:BA:1179:G:C8   | 22:BA:1180:U:O4'  | 2.72                     | 0.43              |
| 22:BA:1208:C:C4   | 22:BA:1209:U:C4   | 3.07                     | 0.43              |
| 22:BA:1248:G:O6   | 26:BE:46:GLN:NE2  | 2.48                     | 0.43              |
| 22:BA:1286:A:N6   | 22:BA:1329:U:C2   | 2.87                     | 0.43              |
| 22:BA:2185:U:C2'  | 22:BA:2186:G:H5'  | 2.49                     | 0.43              |
| 22:BA:2187:U:H2'  | 22:BA:2188:U:O4'  | 2.19                     | 0.43              |
| 22:BA:2323:G:C2'  | 22:BA:2324:U:H5'  | 2.49                     | 0.43              |
| 22:BA:2871:U:OP1  | 35:BN:69:ARG:NH1  | 2.50                     | 0.43              |
| 23:BB:112:G:H2'   | 23:BB:113:C:H6    | 1.84                     | 0.43              |
| 23:BB:43:C:H5''   | 23:BB:44:G:OP2    | 2.19                     | 0.43              |
| 25:BD:149:ASN:OD1 | 25:BD:150:GLN:N   | 2.52                     | 0.43              |
| 28:BG:174:ALA:O   | 28:BG:175:LYS:HB3 | 2.18                     | 0.43              |
| 28:BG:52:PHE:CZ   | 28:BG:72:LEU:HD22 | 2.54                     | 0.43              |
| 36:BO:55:GLU:OE1  | 36:BO:81:ARG:NH1  | 2.50                     | 0.43              |
| 36:BO:94:ARG:HD2  | 36:BO:97:PHE:O    | 2.19                     | 0.43              |
| 43:BV:35:GLU:HB2  | 43:BV:93:ARG:CZ   | 2.49                     | 0.43              |
| 46:BY:6:LEU:HD13  | 46:BY:56:LEU:HD22 | 2.00                     | 0.43              |
| 1:CA:1244:G:C2    | 1:CA:1294:G:C2    | 3.07                     | 0.43              |
| 1:CA:1362:A:OP1   | 1:CA:1362:A:H4'   | 2.19                     | 0.43              |
| 1:CA:1402:C:H2'   | 1:CA:1403:C:O4'   | 2.19                     | 0.43              |
| 1:CA:1435:G:H2'   | 1:CA:1436:U:C6    | 2.54                     | 0.43              |
| 1:CA:1520:C:H2'   | 1:CA:1521:C:C6    | 2.54                     | 0.43              |
| 1:CA:206:C:H2'    | 1:CA:207:C:C4'    | 2.49                     | 0.43              |
| 1:CA:84:U:O2'     | 1:CA:85:U:H5'     | 2.18                     | 0.43              |
| 2:CB:164:ILE:O    | 2:CB:186:ILE:HG23 | 2.19                     | 0.43              |
| 2:CB:21:ARG:HH12  | 2:CB:39:HIS:CD2   | 2.37                     | 0.43              |
| 2:CB:32:PHE:N     | 2:CB:40:ILE:O     | 2.46                     | 0.43              |
| 2:CB:70:VAL:O     | 2:CB:164:ILE:HG22 | 2.18                     | 0.43              |
| 1:CA:439:U:H4'    | 4:CD:121:LYS:HE3  | 2.01                     | 0.43              |
| 7:CG:33:ASP:HB3   | 7:CG:35:LYS:HE3   | 2.00                     | 0.43              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 9:CI:54:LEU:C     | 9:CI:55:VAL:HG13   | 2.39                     | 0.43              |
| 15:CO:46:HIS:O    | 15:CO:48:LYS:N     | 2.41                     | 0.43              |
| 50:D2:9:VAL:HG12  | 50:D2:13:ASN:OD1   | 2.18                     | 0.43              |
| 22:DA:1131:G:N7   | 22:DA:2025:C:H4'   | 2.34                     | 0.43              |
| 22:DA:1358:G:C2'  | 22:DA:1359:A:OP2   | 2.67                     | 0.43              |
| 22:DA:1506:U:H2'  | 22:DA:1507:C:C6    | 2.54                     | 0.43              |
| 22:DA:170:U:C2    | 22:DA:171:U:C6     | 3.07                     | 0.43              |
| 22:DA:1829:A:C8   | 22:DA:1830:C:C5    | 3.07                     | 0.43              |
| 22:DA:1914:C:O2   | 22:DA:1914:C:O4'   | 2.35                     | 0.43              |
| 22:DA:980:A:N6    | 22:DA:2027:G:O2'   | 2.52                     | 0.43              |
| 22:DA:2143:C:H2'  | 22:DA:2144:G:O4'   | 2.19                     | 0.43              |
| 22:DA:2215:C:O2'  | 22:DA:2216:G:H5'   | 2.19                     | 0.43              |
| 22:DA:2314:A:N1   | 22:DA:2315:G:C5    | 2.87                     | 0.43              |
| 22:DA:2379:G:H2'  | 22:DA:2380:C:C6    | 2.54                     | 0.43              |
| 22:DA:2388:A:H5'  | 22:DA:2389:G:OP2   | 2.19                     | 0.43              |
| 22:DA:2473:U:O4   | 28:DG:176:LYS:NZ   | 2.47                     | 0.43              |
| 22:DA:2655:G:O2'  | 22:DA:2656:U:OP1   | 2.30                     | 0.43              |
| 22:DA:2648:G:C4   | 22:DA:2673:G:C2    | 3.06                     | 0.43              |
| 22:DA:2677:G:C4   | 22:DA:2731:G:N2    | 2.87                     | 0.43              |
| 22:DA:2736:A:C2   | 22:DA:2769:U:O2    | 2.71                     | 0.43              |
| 22:DA:2740:A:C6   | 22:DA:2764:A:C8    | 3.07                     | 0.43              |
| 22:DA:729:G:C4    | 22:DA:1775:U:O2    | 2.72                     | 0.43              |
| 22:DA:815:C:H2'   | 22:DA:816:C:C6     | 2.54                     | 0.43              |
| 22:DA:8:C:C2'     | 22:DA:9:G:H5'      | 2.49                     | 0.43              |
| 23:DB:2:G:H8      | 23:DB:2:G:P        | 2.41                     | 0.43              |
| 25:DD:56:LYS:C    | 25:DD:58:ASN:N     | 2.72                     | 0.43              |
| 27:DF:36:LEU:HD23 | 27:DF:57:LEU:HD22  | 2.01                     | 0.43              |
| 29:DH:82:SER:O    | 29:DH:83:LYS:C     | 2.57                     | 0.43              |
| 30:DI:24:VAL:CG1  | 30:DI:28:LEU:HB3   | 2.49                     | 0.43              |
| 30:DI:28:LEU:HD11 | 30:DI:35:ILE:CD1   | 2.49                     | 0.43              |
| 30:DI:8:TYR:HB2   | 30:DI:59:ILE:H     | 1.84                     | 0.43              |
| 30:DI:65:ARG:HG3  | 30:DI:66:SER:N     | 2.32                     | 0.43              |
| 34:DM:107:GLY:C   | 34:DM:108:VAL:HG22 | 2.39                     | 0.43              |
| 22:DA:2873:A:O4'  | 35:DN:6:SER:HB2    | 2.18                     | 0.43              |
| 37:DP:23:GLY:O    | 37:DP:90:GLY:HA3   | 2.19                     | 0.43              |
| 22:DA:973:A:OP2   | 39:DR:81:LYS:HD2   | 2.19                     | 0.43              |
| 39:DR:83:TYR:C    | 39:DR:83:TYR:CD1   | 2.92                     | 0.43              |
| 45:DX:25:THR:O    | 45:DX:27:ARG:N     | 2.52                     | 0.43              |
| 1:AA:1150:A:H2'   | 1:AA:1151:A:H5'    | 2.01                     | 0.43              |
| 1:AA:1225:A:H2'   | 1:AA:1226:C:C6     | 2.53                     | 0.43              |
| 1:AA:1368:A:OP2   | 9:AI:114:LYS:CD    | 2.66                     | 0.43              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:AA:591:U:OP2     | 8:AH:31:LYS:HD2   | 2.18                     | 0.43              |
| 1:AA:639:G:N3      | 1:AA:639:G:H2'    | 2.33                     | 0.43              |
| 1:AA:82:G:O6       | 1:AA:87:C:N4      | 2.52                     | 0.43              |
| 1:AA:947:G:H2'     | 1:AA:948:C:C6     | 2.54                     | 0.43              |
| 2:AB:47:VAL:C      | 2:AB:49:MET:H     | 2.22                     | 0.43              |
| 6:AF:38:ARG:CG     | 6:AF:39:LEU:N     | 2.82                     | 0.43              |
| 8:AH:126:ILE:HG22  | 8:AH:127:CYS:N    | 2.34                     | 0.43              |
| 8:AH:30:SER:O      | 8:AH:31:LYS:C     | 2.58                     | 0.43              |
| 14:AN:13:ARG:O     | 14:AN:17:ALA:HB2  | 2.19                     | 0.43              |
| 14:AN:41:ARG:HB2   | 14:AN:42:TRP:CZ3  | 2.54                     | 0.43              |
| 15:AO:35:GLN:HB3   | 15:AO:59:MET:HE2  | 1.99                     | 0.43              |
| 21:AU:18:ARG:HD2   | 21:AU:18:ARG:H    | 1.84                     | 0.43              |
| 22:BA:100:U:H4'    | 22:BA:101:A:C5'   | 2.49                     | 0.43              |
| 22:BA:1073:A:H2'   | 22:BA:1074:G:H5'' | 2.00                     | 0.43              |
| 22:BA:1097:U:H3'   | 22:BA:1098:A:H4'  | 2.01                     | 0.43              |
| 22:BA:108:G:C2'    | 22:BA:109:C:H5'   | 2.49                     | 0.43              |
| 22:BA:111:A:N1     | 22:BA:112:U:C2    | 2.87                     | 0.43              |
| 22:BA:1406:U:C2'   | 22:BA:1407:G:O5'  | 2.66                     | 0.43              |
| 22:BA:1507:C:H2'   | 22:BA:1508:A:C4'  | 2.49                     | 0.43              |
| 22:BA:1839:G:C2'   | 22:BA:1840:G:O5'  | 2.66                     | 0.43              |
| 22:BA:18:U:O3'     | 38:BQ:23:GLY:HA2  | 2.18                     | 0.43              |
| 22:BA:1972:G:C2    | 22:BA:1973:G:N7   | 2.86                     | 0.43              |
| 22:BA:2192:U:H2'   | 22:BA:2193:G:C5'  | 2.43                     | 0.43              |
| 22:BA:2258:C:O2'   | 22:BA:2426:A:H4'  | 2.19                     | 0.43              |
| 22:BA:2356:U:O3'   | 44:BW:20:ARG:CD   | 2.67                     | 0.43              |
| 22:BA:2564:A:C6    | 22:BA:2565:A:N1   | 2.87                     | 0.43              |
| 22:BA:2684:U:O4'   | 32:BK:70:ARG:NH2  | 2.51                     | 0.43              |
| 22:BA:2838:G:C2'   | 22:BA:2839:G:H5'  | 2.48                     | 0.43              |
| 22:BA:297:G:H2'    | 22:BA:298:G:O4'   | 2.19                     | 0.43              |
| 22:BA:278:A:C6     | 22:BA:362:A:N7    | 2.87                     | 0.43              |
| 22:BA:638:G:C5     | 22:BA:651:G:C2    | 3.07                     | 0.43              |
| 22:BA:830:G:H4'    | 22:BA:831:G:OP2   | 2.19                     | 0.43              |
| 24:BC:22:PRO:C     | 24:BC:24:LEU:H    | 2.23                     | 0.43              |
| 28:BG:141:ILE:HD12 | 28:BG:142:GLY:N   | 2.34                     | 0.43              |
| 31:BJ:30:THR:CG2   | 31:BJ:31:GLU:N    | 2.82                     | 0.43              |
| 22:BA:626:A:C2'    | 33:BL:78:ARG:NH1  | 2.77                     | 0.43              |
| 33:BL:81:ASP:O     | 33:BL:83:ALA:N    | 2.43                     | 0.43              |
| 36:BO:64:TYR:HB3   | 36:BO:67:ASN:ND2  | 2.34                     | 0.43              |
| 39:BR:49:ILE:HG22  | 39:BR:53:PHE:C    | 2.38                     | 0.43              |
| 1:CA:992:U:O4      | 1:CA:1044:A:C8    | 2.72                     | 0.43              |
| 1:CA:1074:G:O2'    | 2:CB:102:THR:HG23 | 2.18                     | 0.43              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:CA:1262:C:N4     | 1:CA:1263:C:N4    | 2.67                     | 0.43              |
| 1:CA:179:A:C5      | 1:CA:180:U:C4     | 3.06                     | 0.43              |
| 1:CA:302:G:C6      | 1:CA:303:A:C5     | 3.07                     | 0.43              |
| 1:CA:314:C:N4      | 1:CA:315:A:N6     | 2.66                     | 0.43              |
| 1:CA:320:A:C2      | 1:CA:334:C:N3     | 2.87                     | 0.43              |
| 1:CA:328:C:O2      | 1:CA:328:C:O2'    | 2.34                     | 0.43              |
| 1:CA:363:A:OP1     | 12:CL:31:ARG:N    | 2.51                     | 0.43              |
| 1:CA:484:G:N7      | 1:CA:486:U:C1'    | 2.82                     | 0.43              |
| 1:CA:978:A:C6      | 1:CA:1318:A:N6    | 2.86                     | 0.43              |
| 3:CC:119:SER:O     | 3:CC:123:GLN:HG3  | 2.19                     | 0.43              |
| 1:CA:1112:C:O2     | 3:CC:179:ARG:HG3  | 2.19                     | 0.43              |
| 3:CC:25:ASN:O      | 3:CC:29:PHE:HB2   | 2.18                     | 0.43              |
| 4:CD:9:LEU:HD22    | 4:CD:22:LYS:HD2   | 2.01                     | 0.43              |
| 5:CE:154:ALA:O     | 5:CE:156:LYS:N    | 2.52                     | 0.43              |
| 5:CE:20:ARG:NH2    | 5:CE:31:PHE:CZ    | 2.87                     | 0.43              |
| 6:CF:37:HIS:O      | 6:CF:97:THR:HG23  | 2.19                     | 0.43              |
| 9:CI:28:ILE:HB     | 9:CI:35:LEU:HB2   | 2.01                     | 0.43              |
| 9:CI:49:ARG:C      | 9:CI:51:PRO:HD2   | 2.38                     | 0.43              |
| 10:CJ:27:GLU:O     | 10:CJ:31:ARG:HB3  | 2.18                     | 0.43              |
| 12:CL:44:LYS:HB3   | 12:CL:45:PRO:CD   | 2.48                     | 0.43              |
| 13:CM:48:LEU:HD22  | 13:CM:53:ILE:HG13 | 2.01                     | 0.43              |
| 13:CM:64:VAL:O     | 13:CM:69:LEU:HB2  | 2.18                     | 0.43              |
| 14:CN:25:ALA:O     | 14:CN:28:LYS:HG2  | 2.19                     | 0.43              |
| 14:CN:64:CYS:SG    | 14:CN:83:LYS:HG3  | 2.59                     | 0.43              |
| 16:CP:6:LEU:CD1    | 16:CP:71:VAL:HG23 | 2.49                     | 0.43              |
| 1:CA:957:U:H4'     | 19:CS:79:THR:O    | 2.19                     | 0.43              |
| 21:CU:34:ARG:HD3   | 21:CU:35:ARG:HB3  | 2.00                     | 0.43              |
| 22:DA:1304:A:C6    | 22:DA:1305:C:N4   | 2.87                     | 0.43              |
| 22:DA:1357:C:C2'   | 22:DA:1358:G:H5'  | 2.49                     | 0.43              |
| 22:DA:1662:U:O2    | 22:DA:2687:U:H4'  | 2.19                     | 0.43              |
| 22:DA:1765:U:O2'   | 22:DA:1766:G:H5'  | 2.19                     | 0.43              |
| 22:DA:1884:G:O2'   | 22:DA:1885:A:OP2  | 2.34                     | 0.43              |
| 22:DA:192:C:C4     | 22:DA:193:U:C2    | 3.07                     | 0.43              |
| 22:DA:2021:C:OP1   | 48:D0:9:THR:HG21  | 2.19                     | 0.43              |
| 22:DA:2332:C:H4'   | 22:DA:2336:A:H62  | 1.84                     | 0.43              |
| 22:DA:2511:U:C4    | 22:DA:2512:C:C4   | 3.07                     | 0.43              |
| 22:DA:290:U:N3     | 22:DA:291:G:N7    | 2.67                     | 0.43              |
| 22:DA:303:G:C2     | 22:DA:315:G:C6    | 3.07                     | 0.43              |
| 22:DA:232:G:N2     | 22:DA:420:C:OP1   | 2.51                     | 0.43              |
| 22:DA:753:A:H2'    | 22:DA:754:U:C6    | 2.54                     | 0.43              |
| 25:DD:122:VAL:HG21 | 25:DD:141:ARG:NH1 | 2.34                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 25:DD:14:ILE:HG12 | 25:DD:24:VAL:CG2  | 2.49                     | 0.43              |
| 27:DF:66:LEU:O    | 27:DF:87:CYS:HA   | 2.19                     | 0.43              |
| 30:DI:91:GLY:O    | 30:DI:93:PRO:HD3  | 2.19                     | 0.43              |
| 31:DJ:59:ALA:O    | 31:DJ:62:VAL:CG1  | 2.67                     | 0.43              |
| 35:DN:38:LEU:N    | 35:DN:39:PRO:CD   | 2.82                     | 0.43              |
| 40:DS:61:ASN:O    | 40:DS:62:ASP:OD1  | 2.37                     | 0.43              |
| 42:DU:74:ASN:O    | 42:DU:75:ALA:HB3  | 2.18                     | 0.43              |
| 45:DX:27:ARG:NE   | 45:DX:28:ARG:O    | 2.50                     | 0.43              |
| 1:AA:1031:C:O2'   | 1:AA:1032:G:P     | 2.77                     | 0.42              |
| 1:AA:1181:G:H4'   | 1:AA:1182:G:OP1   | 2.18                     | 0.42              |
| 1:AA:1233:G:OP1   | 9:AI:126:GLN:HB3  | 2.19                     | 0.42              |
| 1:AA:1310:G:O2'   | 1:AA:1311:A:H5'   | 2.18                     | 0.42              |
| 1:AA:131:A:C2     | 1:AA:132:C:C4     | 3.07                     | 0.42              |
| 1:AA:160:A:N6     | 1:AA:347:G:H1'    | 2.34                     | 0.42              |
| 1:AA:448:A:C5     | 1:AA:487:A:C2     | 3.07                     | 0.42              |
| 1:AA:670:G:H2'    | 1:AA:671:G:O5'    | 2.18                     | 0.42              |
| 1:AA:83:C:H2'     | 1:AA:85:U:OP2     | 2.18                     | 0.42              |
| 1:AA:958:A:C6     | 1:AA:959:A:N1     | 2.87                     | 0.42              |
| 2:AB:147:SER:O    | 2:AB:148:LEU:CG   | 2.67                     | 0.42              |
| 3:AC:110:GLU:HG2  | 3:AC:140:ASN:HB3  | 2.01                     | 0.42              |
| 4:AD:157:ALA:O    | 4:AD:161:LEU:HD22 | 2.19                     | 0.42              |
| 4:AD:167:LYS:O    | 4:AD:168:PRO:O    | 2.37                     | 0.42              |
| 6:AF:71:ILE:HG23  | 6:AF:72:ASP:N     | 2.33                     | 0.42              |
| 12:AL:67:ILE:HG21 | 12:AL:72:HIS:CD2  | 2.54                     | 0.42              |
| 13:AM:80:LEU:HD21 | 13:AM:87:ARG:NE   | 2.34                     | 0.42              |
| 15:AO:62:GLN:O    | 15:AO:63:ARG:C    | 2.57                     | 0.42              |
| 19:AS:34:TRP:O    | 19:AS:36:ARG:N    | 2.52                     | 0.42              |
| 20:AT:44:LYS:HD3  | 20:AT:87:ALA:HA   | 2.01                     | 0.42              |
| 53:B5:208:THR:O   | 53:B5:209:PHE:CB  | 2.67                     | 0.42              |
| 22:BA:1253:A:C8   | 57:BA:3337:HOH:O  | 2.72                     | 0.42              |
| 22:BA:1515:A:H2'  | 22:BA:1516:G:O4'  | 2.19                     | 0.42              |
| 22:BA:1535:A:H5'  | 22:BA:1536:C:C5   | 2.55                     | 0.42              |
| 22:BA:164:C:H2'   | 22:BA:165:A:O4'   | 2.18                     | 0.42              |
| 22:BA:2308:G:C6   | 22:BA:2311:A:N7   | 2.87                     | 0.42              |
| 22:BA:2436:G:C2   | 22:BA:2437:G:C8   | 3.07                     | 0.42              |
| 22:BA:2577:A:C2'  | 22:BA:2578:G:OP1  | 2.67                     | 0.42              |
| 22:BA:263:G:H2'   | 22:BA:264:C:C5'   | 2.49                     | 0.42              |
| 22:BA:2:G:H2'     | 22:BA:3:U:C6      | 2.54                     | 0.42              |
| 22:BA:685:A:H1'   | 22:BA:688:U:O4    | 2.19                     | 0.42              |
| 22:BA:846:U:HO2'  | 22:BA:847:U:P     | 2.39                     | 0.42              |
| 24:BC:201:MET:HG3 | 24:BC:202:LEU:CD1 | 2.49                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 25:BD:119:ALA:HB2 | 25:BD:165:MET:HG2  | 2.00                     | 0.42              |
| 26:BE:77:ILE:HG13 | 26:BE:77:ILE:O     | 2.19                     | 0.42              |
| 22:BA:471:A:H5'   | 26:BE:79:ARG:NH2   | 2.34                     | 0.42              |
| 29:BH:79:THR:CG2  | 29:BH:147:VAL:CG2  | 2.97                     | 0.42              |
| 30:BI:39:CYS:O    | 30:BI:42:PHE:HB3   | 2.19                     | 0.42              |
| 33:BL:82:LEU:C    | 33:BL:84:LYS:H     | 2.22                     | 0.42              |
| 39:BR:51:VAL:CG2  | 39:BR:52:PRO:HD2   | 2.49                     | 0.42              |
| 39:BR:74:ILE:HD13 | 39:BR:74:ILE:N     | 2.34                     | 0.42              |
| 1:CA:108:G:C6     | 20:CT:10:ARG:HG2   | 2.54                     | 0.42              |
| 1:CA:1134:G:C6    | 1:CA:1141:C:N4     | 2.87                     | 0.42              |
| 1:CA:124:C:N4     | 1:CA:125:U:O4      | 2.52                     | 0.42              |
| 1:CA:1317:C:H2'   | 1:CA:1318:A:O5'    | 2.19                     | 0.42              |
| 1:CA:1537:U:C5    | 1:CA:1538:C:N4     | 2.87                     | 0.42              |
| 1:CA:392:C:C2     | 1:CA:393:A:C8      | 3.07                     | 0.42              |
| 1:CA:411:A:H4'    | 1:CA:412:A:O5'     | 2.18                     | 0.42              |
| 1:CA:793:U:HO2'   | 1:CA:1516:G:C2'    | 2.29                     | 0.42              |
| 1:CA:81:A:N1      | 1:CA:88:U:O4       | 2.52                     | 0.42              |
| 2:CB:140:GLU:O    | 2:CB:141:LEU:C     | 2.56                     | 0.42              |
| 4:CD:170:TRP:O    | 4:CD:183:LYS:HB2   | 2.19                     | 0.42              |
| 4:CD:142:VAL:CG1  | 4:CD:181:THR:OG1   | 2.67                     | 0.42              |
| 4:CD:90:LEU:CD2   | 4:CD:200:ILE:HD11  | 2.49                     | 0.42              |
| 7:CG:51:ALA:HB2   | 7:CG:58:GLU:HA     | 2.00                     | 0.42              |
| 10:CJ:17:LEU:HD21 | 10:CJ:96:VAL:HG22  | 2.00                     | 0.42              |
| 14:CN:21:PHE:CD2  | 14:CN:25:ALA:HB2   | 2.54                     | 0.42              |
| 17:CQ:21:ILE:HB   | 17:CQ:48:ASP:OD1   | 2.18                     | 0.42              |
| 18:CR:33:ILE:CA   | 18:CR:40:VAL:HG23  | 2.47                     | 0.42              |
| 21:CU:26:ALA:O    | 21:CU:27:GLY:C     | 2.56                     | 0.42              |
| 52:D4:7:VAL:HG13  | 52:D4:38:GLY:CA    | 2.49                     | 0.42              |
| 22:DA:1462:C:C2   | 22:DA:1463:C:C5    | 3.07                     | 0.42              |
| 22:DA:158:U:O4    | 22:DA:159:G:C6     | 2.72                     | 0.42              |
| 22:DA:324:A:C6    | 22:DA:325:G:C4     | 3.06                     | 0.42              |
| 22:DA:109:C:H5'   | 22:DA:348:A:C4'    | 2.49                     | 0.42              |
| 22:DA:447:A:O2'   | 22:DA:473:G:N7     | 2.40                     | 0.42              |
| 22:DA:597:G:C6    | 22:DA:598:U:C2     | 3.07                     | 0.42              |
| 22:DA:600:G:OP1   | 26:DE:24:ASN:ND2   | 2.48                     | 0.42              |
| 22:DA:683:U:OP1   | 50:D2:26:ASN:CB    | 2.67                     | 0.42              |
| 22:DA:779:U:OP1   | 24:DC:49:ILE:HG13  | 2.19                     | 0.42              |
| 25:DD:109:VAL:CG1 | 25:DD:201:LEU:HD22 | 2.48                     | 0.42              |
| 26:DE:131:THR:O   | 26:DE:135:ALA:HB2  | 2.19                     | 0.42              |
| 27:DF:110:ARG:CZ  | 27:DF:110:ARG:HB3  | 2.49                     | 0.42              |
| 22:DA:2311:A:H2   | 27:DF:79:ILE:CG2   | 2.31                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 30:DI:10:LYS:HB2   | 30:DI:56:PRO:HB2   | 2.01                     | 0.42              |
| 39:DR:64:VAL:O     | 39:DR:65:ALA:HB2   | 2.19                     | 0.42              |
| 41:DT:4:GLU:O      | 41:DT:8:LEU:N      | 2.51                     | 0.42              |
| 43:DV:75:GLN:CB    | 43:DV:92:VAL:HG23  | 2.49                     | 0.42              |
| 1:AA:1012:A:C2     | 1:AA:1018:G:N7     | 2.87                     | 0.42              |
| 1:AA:1182:G:C3'    | 1:AA:1183:U:H5'    | 2.49                     | 0.42              |
| 1:AA:1264:U:O2     | 1:AA:1272:G:C2     | 2.71                     | 0.42              |
| 1:AA:1418:A:N6     | 1:AA:1482:G:O2'    | 2.46                     | 0.42              |
| 1:AA:209:U:C4'     | 1:AA:210:C:OP2     | 2.64                     | 0.42              |
| 1:AA:292:G:O2'     | 1:AA:608:A:N6      | 2.52                     | 0.42              |
| 1:AA:28:A:C6       | 1:AA:29:U:N3       | 2.87                     | 0.42              |
| 1:AA:760:G:C8      | 1:AA:761:G:C8      | 3.07                     | 0.42              |
| 1:AA:812:G:OP1     | 1:AA:903:G:H1'     | 2.18                     | 0.42              |
| 1:AA:959:A:N7      | 1:AA:960:U:C6      | 2.87                     | 0.42              |
| 3:AC:141:ALA:O     | 3:AC:146:ALA:HB3   | 2.18                     | 0.42              |
| 4:AD:188:ARG:O     | 4:AD:190:ASP:O     | 2.37                     | 0.42              |
| 4:AD:76:TYR:O      | 4:AD:77:LYS:C      | 2.57                     | 0.42              |
| 4:AD:97:ARG:HB3    | 4:AD:99:ASP:OD1    | 2.19                     | 0.42              |
| 5:AE:115:LEU:HG    | 5:AE:120:VAL:HG21  | 2.01                     | 0.42              |
| 5:AE:39:VAL:HG22   | 5:AE:67:ALA:HB1    | 2.00                     | 0.42              |
| 8:AH:64:LYS:HB3    | 8:AH:71:VAL:HG21   | 2.01                     | 0.42              |
| 1:AA:1359:C:P      | 14:AN:62:ASN:HD22  | 2.43                     | 0.42              |
| 16:AP:53:ASP:OD1   | 16:AP:53:ASP:O     | 2.37                     | 0.42              |
| 19:AS:37:ARG:O     | 19:AS:70:LYS:HD2   | 2.18                     | 0.42              |
| 53:B5:66:PRO:O     | 53:B5:190:ILE:CB   | 2.67                     | 0.42              |
| 22:BA:102:U:C4     | 46:BY:2:LYS:HD2    | 2.55                     | 0.42              |
| 22:BA:1070:A:C2    | 22:BA:1097:U:O2'   | 2.68                     | 0.42              |
| 22:BA:1140:C:OP2   | 31:BJ:68:LYS:NZ    | 2.45                     | 0.42              |
| 22:BA:1299:G:O2'   | 22:BA:1301:A:N7    | 2.50                     | 0.42              |
| 22:BA:2190:G:C2'   | 22:BA:2191:A:H5'   | 2.49                     | 0.42              |
| 22:BA:2298:A:N6    | 22:BA:2318:G:H1'   | 2.34                     | 0.42              |
| 22:BA:2500:U:O2    | 22:BA:2504:U:C4    | 2.72                     | 0.42              |
| 22:BA:2727:A:C6    | 22:BA:2728:U:O4    | 2.72                     | 0.42              |
| 22:BA:418:C:H2'    | 22:BA:419:U:O4'    | 2.19                     | 0.42              |
| 22:BA:511:U:O4     | 22:BA:512:G:N1     | 2.52                     | 0.42              |
| 22:BA:734:A:C5     | 22:BA:735:A:C8     | 3.07                     | 0.42              |
| 22:BA:866:A:N7     | 22:BA:914:G:C6     | 2.88                     | 0.42              |
| 22:BA:991:C:C2     | 22:BA:1185:G:N1    | 2.87                     | 0.42              |
| 27:BF:3:LYS:HB3    | 27:BF:101:GLU:OE1  | 2.19                     | 0.42              |
| 27:BF:105:THR:HG23 | 27:BF:106:ILE:HG12 | 2.01                     | 0.42              |
| 30:BI:72:LYS:N     | 30:BI:72:LYS:CD    | 2.82                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 33:BL:26:GLY:C   | 33:BL:27:LEU:HD23 | 2.40                     | 0.42              |
| 33:BL:29:LYS:HB3 | 33:BL:30:THR:H    | 1.70                     | 0.42              |
| 35:BN:77:ALA:O   | 35:BN:81:ASN:HB2  | 2.19                     | 0.42              |
| 40:BS:28:LYS:O   | 40:BS:29:VAL:C    | 2.57                     | 0.42              |
| 1:CA:1115:U:O2   | 1:CA:1186:G:C2    | 2.72                     | 0.42              |
| 1:CA:1179:A:H2'  | 1:CA:1180:A:O4'   | 2.19                     | 0.42              |
| 1:CA:954:G:C2    | 1:CA:1228:C:N3    | 2.87                     | 0.42              |
| 1:CA:158:G:C6    | 1:CA:164:G:C5     | 3.07                     | 0.42              |
| 1:CA:6:G:H4'     | 1:CA:298:A:H4'    | 2.01                     | 0.42              |
| 1:CA:297:G:N2    | 1:CA:300:A:OP2    | 2.47                     | 0.42              |
| 1:CA:405:U:OP2   | 4:CD:3:ARG:NH1    | 2.52                     | 0.42              |
| 1:CA:466:A:C2    | 1:CA:468:A:N7     | 2.88                     | 0.42              |
| 1:CA:519:C:C4    | 1:CA:520:A:C6     | 3.07                     | 0.42              |
| 1:CA:542:G:C2    | 1:CA:543:U:C6     | 3.08                     | 0.42              |
| 1:CA:552:U:N3    | 1:CA:553:A:N7     | 2.67                     | 0.42              |
| 1:CA:671:G:C2    | 1:CA:672:U:C2     | 3.07                     | 0.42              |
| 1:CA:866:C:C4    | 1:CA:867:G:H1'    | 2.54                     | 0.42              |
| 1:CA:959:A:C2    | 1:CA:1222:G:O4'   | 2.72                     | 0.42              |
| 1:CA:978:A:P     | 1:CA:1362:A:N6    | 2.92                     | 0.42              |
| 2:CB:25:PRO:O    | 2:CB:28:LYS:HB2   | 2.19                     | 0.42              |
| 3:CC:40:ARG:NH1  | 3:CC:55:ILE:HG13  | 2.34                     | 0.42              |
| 6:CF:92:THR:HG22 | 6:CF:93:LYS:N     | 2.34                     | 0.42              |
| 9:CI:47:VAL:O    | 9:CI:80:ARG:HG3   | 2.19                     | 0.42              |
| 13:CM:22:ILE:HB  | 13:CM:25:VAL:HG12 | 2.00                     | 0.42              |
| 14:CN:31:ILE:N   | 14:CN:31:ILE:HD12 | 2.34                     | 0.42              |
| 15:CO:67:LEU:O   | 15:CO:70:LEU:N    | 2.52                     | 0.42              |
| 17:CQ:15:ASP:HA  | 17:CQ:21:ILE:HD12 | 2.01                     | 0.42              |
| 19:CS:66:MET:O   | 19:CS:68:GLY:N    | 2.53                     | 0.42              |
| 22:DA:1264:A:N7  | 22:DA:1265:A:C5   | 2.87                     | 0.42              |
| 22:DA:1361:G:C6  | 22:DA:1371:G:C2   | 3.07                     | 0.42              |
| 22:DA:1394:U:H3' | 22:DA:1394:U:H6   | 1.84                     | 0.42              |
| 22:DA:1525:A:H2' | 22:DA:1526:C:O4'  | 2.19                     | 0.42              |
| 22:DA:1680:U:H2' | 22:DA:1681:G:O4'  | 2.19                     | 0.42              |
| 22:DA:1857:G:N2  | 22:DA:1884:G:C4   | 2.87                     | 0.42              |
| 22:DA:1875:G:H2' | 22:DA:1876:A:OP2  | 2.19                     | 0.42              |
| 22:DA:2013:A:N1  | 22:DA:2014:A:C2   | 2.87                     | 0.42              |
| 22:DA:2098:U:C4  | 22:DA:2099:U:O4   | 2.72                     | 0.42              |
| 22:DA:965:C:C4'  | 22:DA:2273:A:H1'  | 2.49                     | 0.42              |
| 22:DA:2289:G:O2' | 22:DA:2383:G:O2'  | 2.32                     | 0.42              |
| 22:DA:237:C:C4   | 22:DA:238:C:H5    | 2.36                     | 0.42              |
| 22:DA:249:C:P    | 22:DA:2394:C:O2'  | 2.77                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:DA:2587:A:H5''  | 22:DA:2588:G:OP2   | 2.20                     | 0.42              |
| 22:DA:426:C:C4     | 22:DA:427:U:C5     | 3.07                     | 0.42              |
| 23:DB:96:G:O2'     | 23:DB:97:C:H5'     | 2.19                     | 0.42              |
| 24:DC:17:VAL:N     | 24:DC:204:VAL:HG22 | 2.34                     | 0.42              |
| 26:DE:149:ILE:HG22 | 26:DE:186:VAL:HG12 | 2.00                     | 0.42              |
| 30:DI:54:PRO:O     | 30:DI:75:PRO:HD2   | 2.18                     | 0.42              |
| 23:DB:90:C:H5'     | 34:DM:18:ARG:HG2   | 2.01                     | 0.42              |
| 35:DN:2:ARG:CD     | 35:DN:2:ARG:O      | 2.68                     | 0.42              |
| 35:DN:47:VAL:O     | 35:DN:47:VAL:HG12  | 2.19                     | 0.42              |
| 37:DP:114:LEU:HG   | 37:DP:114:LEU:O    | 2.20                     | 0.42              |
| 22:DA:1250:G:H4'   | 38:DQ:6:ARG:HD2    | 2.01                     | 0.42              |
| 39:DR:80:ARG:C     | 39:DR:82:HIS:N     | 2.72                     | 0.42              |
| 41:DT:24:MET:HG2   | 41:DT:29:THR:O     | 2.19                     | 0.42              |
| 42:DU:49:VAL:HG13  | 42:DU:53:ASN:O     | 2.19                     | 0.42              |
| 1:AA:1538:C:O2'    | 1:AA:1539:C:H5'    | 2.19                     | 0.42              |
| 1:AA:172:A:C5      | 1:AA:174:A:C8      | 3.08                     | 0.42              |
| 1:AA:457:G:N3      | 1:AA:457:G:H2'     | 2.34                     | 0.42              |
| 1:AA:939:G:C2      | 1:AA:940:C:C2      | 3.07                     | 0.42              |
| 2:AB:20:THR:O      | 2:AB:21:ARG:NH2    | 2.53                     | 0.42              |
| 3:AC:85:GLU:O      | 3:AC:87:LEU:N      | 2.52                     | 0.42              |
| 5:AE:94:VAL:HG21   | 5:AE:140:THR:HG22  | 2.00                     | 0.42              |
| 6:AF:99:ALA:O      | 6:AF:100:SER:CB    | 2.67                     | 0.42              |
| 8:AH:78:VAL:HG11   | 8:AH:125:ILE:HD11  | 2.00                     | 0.42              |
| 11:AK:35:THR:CG2   | 11:AK:39:GLY:HA2   | 2.49                     | 0.42              |
| 13:AM:6:GLY:C      | 13:AM:8:ASN:N      | 2.70                     | 0.42              |
| 49:B1:12:VAL:HG12  | 49:B1:13:SER:N     | 2.34                     | 0.42              |
| 52:B4:10:LEU:N     | 52:B4:14:CYS:SG    | 2.80                     | 0.42              |
| 22:BA:1064:C:H4'   | 30:BI:90:SER:CB    | 2.48                     | 0.42              |
| 22:BA:122:G:H2'    | 22:BA:123:G:O4'    | 2.19                     | 0.42              |
| 22:BA:1283:G:N1    | 22:BA:1286:A:OP2   | 2.53                     | 0.42              |
| 22:BA:1353:A:C8    | 22:BA:1378:A:N6    | 2.88                     | 0.42              |
| 22:BA:1449:G:C6    | 22:BA:1450:G:N7    | 2.88                     | 0.42              |
| 22:BA:1738:G:HO2'  | 22:BA:1739:A:P     | 2.43                     | 0.42              |
| 22:BA:1847:A:C8    | 22:BA:1847:A:OP2   | 2.73                     | 0.42              |
| 22:BA:2214:C:H2'   | 22:BA:2215:C:O4'   | 2.19                     | 0.42              |
| 22:BA:2748:A:C2    | 22:BA:2757:A:C4    | 3.07                     | 0.42              |
| 22:BA:301:G:C6     | 22:BA:317:G:C6     | 3.07                     | 0.42              |
| 22:BA:476:G:C2     | 22:BA:479:A:C8     | 3.07                     | 0.42              |
| 22:BA:644:A:H5''   | 22:BA:645:C:OP2    | 2.18                     | 0.42              |
| 24:BC:75:PRO:HA    | 24:BC:117:GLN:HG2  | 2.00                     | 0.42              |
| 22:BA:1805:A:N3    | 24:BC:50:THR:HB    | 2.33                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 28:BG:96:ALA:HB2   | 28:BG:105:LEU:HD23 | 2.02                     | 0.42              |
| 30:BI:16:GLY:CA    | 30:BI:51:LYS:HB3   | 2.49                     | 0.42              |
| 22:BA:1277:G:C5'   | 35:BN:20:MET:CE    | 2.97                     | 0.42              |
| 35:BN:36:THR:HG23  | 35:BN:37:THR:O     | 2.19                     | 0.42              |
| 23:BB:116:G:C4'    | 36:BO:54:VAL:HG13  | 2.46                     | 0.42              |
| 37:BP:103:ARG:HH11 | 37:BP:103:ARG:HG2  | 1.83                     | 0.42              |
| 39:BR:2:TYR:HA     | 39:BR:14:VAL:O     | 2.20                     | 0.42              |
| 40:BS:109:ASP:O    | 40:BS:110:ARG:O    | 2.37                     | 0.42              |
| 42:BU:39:ILE:HG22  | 42:BU:40:ASN:N     | 2.34                     | 0.42              |
| 1:CA:1000:A:N3     | 1:CA:1041:G:N2     | 2.67                     | 0.42              |
| 1:CA:1087:G:N2     | 1:CA:1099:G:H1'    | 2.35                     | 0.42              |
| 1:CA:1144:G:N2     | 1:CA:1145:A:C2     | 2.87                     | 0.42              |
| 1:CA:1362:A:OP1    | 1:CA:1362:A:C4'    | 2.67                     | 0.42              |
| 1:CA:189:A:N7      | 1:CA:190:A:C5      | 2.88                     | 0.42              |
| 1:CA:244:U:O4      | 1:CA:906:A:H1'     | 2.18                     | 0.42              |
| 1:CA:270:A:H2'     | 1:CA:271:C:C6      | 2.54                     | 0.42              |
| 1:CA:456:A:H2'     | 1:CA:457:G:O4'     | 2.19                     | 0.42              |
| 1:CA:623:C:C4      | 1:CA:624:C:C5      | 3.07                     | 0.42              |
| 1:CA:662:U:H2'     | 1:CA:663:A:C8      | 2.55                     | 0.42              |
| 1:CA:853:C:C2      | 1:CA:854:U:C6      | 3.06                     | 0.42              |
| 2:CB:21:ARG:HA     | 2:CB:21:ARG:NE     | 2.32                     | 0.42              |
| 6:CF:3:HIS:O       | 6:CF:92:THR:HA     | 2.19                     | 0.42              |
| 11:CK:116:ILE:O    | 11:CK:116:ILE:HG22 | 2.19                     | 0.42              |
| 13:CM:4:ILE:HG22   | 13:CM:53:ILE:CG2   | 2.48                     | 0.42              |
| 14:CN:87:ALA:HB1   | 14:CN:92:GLU:CB    | 2.49                     | 0.42              |
| 16:CP:42:ILE:O     | 16:CP:43:ALA:HB3   | 2.19                     | 0.42              |
| 20:CT:84:ASN:O     | 20:CT:84:ASN:ND2   | 2.53                     | 0.42              |
| 21:CU:14:VAL:CG1   | 21:CU:15:ALA:N     | 2.82                     | 0.42              |
| 22:DA:110:G:N2     | 22:DA:111:A:H1'    | 2.35                     | 0.42              |
| 22:DA:121:G:N2     | 22:DA:131:A:C4     | 2.88                     | 0.42              |
| 22:DA:1267:U:C5    | 22:DA:2012:G:N2    | 2.88                     | 0.42              |
| 22:DA:1298:C:N4    | 22:DA:1299:G:C6    | 2.87                     | 0.42              |
| 22:DA:1355:G:N1    | 22:DA:1356:G:C8    | 2.88                     | 0.42              |
| 22:DA:1361:G:N3    | 22:DA:1362:C:C6    | 2.87                     | 0.42              |
| 22:DA:1553:A:N7    | 22:DA:1555:G:C5    | 2.87                     | 0.42              |
| 22:DA:1607:C:H4'   | 22:DA:1608:A:C5'   | 2.49                     | 0.42              |
| 22:DA:1858:A:C6    | 22:DA:1859:U:N3    | 2.87                     | 0.42              |
| 22:DA:2096:C:H2'   | 22:DA:2097:A:C8    | 2.54                     | 0.42              |
| 22:DA:2225:A:H1'   | 22:DA:2226:C:OP2   | 2.20                     | 0.42              |
| 22:DA:2393:U:H2'   | 22:DA:2394:C:O4'   | 2.20                     | 0.42              |
| 22:DA:927:A:H2'    | 22:DA:928:A:O4'    | 2.19                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 23:DB:94:A:C2'    | 23:DB:95:U:H5'    | 2.49                     | 0.42              |
| 25:DD:14:ILE:HG12 | 25:DD:24:VAL:HG21 | 2.01                     | 0.42              |
| 30:DI:46:THR:HG22 | 30:DI:51:LYS:HG3  | 2.01                     | 0.42              |
| 22:DA:538:A:H5''  | 31:DJ:7:LYS:NZ    | 2.35                     | 0.42              |
| 35:DN:76:VAL:HA   | 35:DN:79:LEU:HD12 | 2.01                     | 0.42              |
| 43:DV:80:HIS:CG   | 43:DV:81:PRO:HD2  | 2.55                     | 0.42              |
| 46:DY:29:ARG:C    | 46:DY:31:GLN:H    | 2.22                     | 0.42              |
| 1:AA:1270:G:O3'   | 1:AA:1314:C:H5'   | 2.19                     | 0.42              |
| 1:AA:1359:C:H2'   | 1:AA:1361:G:OP2   | 2.20                     | 0.42              |
| 1:AA:1468:A:O2'   | 1:AA:1469:C:H5'   | 2.19                     | 0.42              |
| 1:AA:328:C:C2'    | 1:AA:328:C:O2     | 2.68                     | 0.42              |
| 1:AA:764:C:O2'    | 1:AA:765:G:H5'    | 2.19                     | 0.42              |
| 1:AA:694:A:N1     | 1:AA:787:A:O2'    | 2.52                     | 0.42              |
| 7:AG:49:THR:O     | 7:AG:53:ARG:HB2   | 2.18                     | 0.42              |
| 7:AG:91:VAL:O     | 7:AG:96:ARG:NH2   | 2.53                     | 0.42              |
| 1:AA:1178:G:C8    | 9:AI:99:ARG:NH2   | 2.87                     | 0.42              |
| 10:AJ:67:ILE:HG22 | 10:AJ:67:ILE:O    | 2.19                     | 0.42              |
| 10:AJ:80:THR:C    | 10:AJ:82:LYS:H    | 2.22                     | 0.42              |
| 11:AK:16:VAL:HG13 | 11:AK:17:SER:H    | 1.84                     | 0.42              |
| 13:AM:45:ILE:HG13 | 13:AM:48:LEU:HD13 | 2.01                     | 0.42              |
| 18:AR:71:THR:OG1  | 18:AR:73:ARG:N    | 2.50                     | 0.42              |
| 20:AT:79:LEU:O    | 20:AT:82:GLN:HB2  | 2.19                     | 0.42              |
| 53:B5:23:ILE:HG22 | 53:B5:23:ILE:O    | 2.20                     | 0.42              |
| 22:BA:1122:G:N3   | 22:BA:1122:G:H2'  | 2.33                     | 0.42              |
| 22:BA:141:G:C6    | 41:BT:1:MET:HE1   | 2.54                     | 0.42              |
| 22:BA:1447:C:H1'  | 22:BA:1545:A:H1'  | 2.01                     | 0.42              |
| 22:BA:1439:A:C2   | 22:BA:1553:A:C6   | 3.07                     | 0.42              |
| 22:BA:1692:U:H2'  | 22:BA:1694:C:C5   | 2.54                     | 0.42              |
| 22:BA:189:G:H2'   | 22:BA:205:G:N2    | 2.35                     | 0.42              |
| 22:BA:196:A:H2'   | 22:BA:196:A:N3    | 2.34                     | 0.42              |
| 22:BA:2271:G:H2'  | 22:BA:2272:U:C6   | 2.55                     | 0.42              |
| 22:BA:2315:G:H2'  | 22:BA:2316:G:H8   | 1.83                     | 0.42              |
| 22:BA:2674:G:H4'  | 32:BK:30:ARG:HD2  | 2.02                     | 0.42              |
| 22:BA:464:U:C5    | 22:BA:788:A:C4    | 3.08                     | 0.42              |
| 22:BA:82:U:H2'    | 22:BA:83:A:O4'    | 2.19                     | 0.42              |
| 22:BA:996:A:C5    | 22:BA:1160:G:C2   | 3.08                     | 0.42              |
| 24:BC:78:VAL:HG21 | 24:BC:110:LEU:CD2 | 2.49                     | 0.42              |
| 24:BC:237:GLY:HA3 | 57:BC:407:HOH:O   | 2.19                     | 0.42              |
| 26:BE:141:MET:O   | 26:BE:142:ALA:HB3 | 2.19                     | 0.42              |
| 27:BF:95:ARG:HA   | 27:BF:98:GLU:HB2  | 2.02                     | 0.42              |
| 31:BJ:53:TYR:CD1  | 31:BJ:121:LYS:HB3 | 2.55                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 32:BK:25:LEU:HD12 | 32:BK:38:ILE:HG22  | 2.01                     | 0.42              |
| 35:BN:116:VAL:O   | 35:BN:116:VAL:HG13 | 2.19                     | 0.42              |
| 38:BQ:25:TYR:O    | 38:BQ:26:GLY:C     | 2.57                     | 0.42              |
| 41:BT:44:LYS:HG3  | 41:BT:55:VAL:CG1   | 2.50                     | 0.42              |
| 42:BU:97:LYS:O    | 42:BU:98:SER:CB    | 2.67                     | 0.42              |
| 46:BY:22:LEU:O    | 46:BY:23:ARG:O     | 2.37                     | 0.42              |
| 46:BY:7:ARG:HG3   | 46:BY:7:ARG:O      | 2.20                     | 0.42              |
| 1:CA:47:C:H4'     | 1:CA:48:C:OP1      | 2.20                     | 0.42              |
| 1:CA:57:G:H2'     | 1:CA:58:C:C6       | 2.55                     | 0.42              |
| 2:CB:86:SER:O     | 2:CB:87:CYS:O      | 2.36                     | 0.42              |
| 3:CC:141:ALA:O    | 3:CC:146:ALA:HB3   | 2.18                     | 0.42              |
| 3:CC:147:LYS:HB2  | 3:CC:203:PHE:CD2   | 2.54                     | 0.42              |
| 4:CD:145:ILE:HG22 | 4:CD:146:ARG:O     | 2.19                     | 0.42              |
| 7:CG:130:ASN:HA   | 7:CG:135:VAL:HG11  | 2.00                     | 0.42              |
| 7:CG:40:GLU:HA    | 7:CG:43:VAL:HB     | 2.01                     | 0.42              |
| 11:CK:127:ARG:O   | 21:CU:34:ARG:NH1   | 2.40                     | 0.42              |
| 12:CL:30:LYS:O    | 12:CL:81:LEU:HD12  | 2.19                     | 0.42              |
| 1:CA:1317:C:C4    | 14:CN:53:ARG:HD2   | 2.54                     | 0.42              |
| 17:CQ:46:VAL:HG11 | 17:CQ:61:ILE:CG1   | 2.49                     | 0.42              |
| 18:CR:57:ARG:HG2  | 18:CR:58:ALA:N     | 2.34                     | 0.42              |
| 19:CS:44:MET:HE1  | 19:CS:71:LEU:HD21  | 2.00                     | 0.42              |
| 20:CT:58:VAL:CG1  | 20:CT:72:ALA:HB1   | 2.49                     | 0.42              |
| 20:CT:69:LYS:HD2  | 20:CT:70:ASN:OD1   | 2.19                     | 0.42              |
| 21:CU:11:PRO:C    | 21:CU:12:PHE:CG    | 2.93                     | 0.42              |
| 50:D2:9:VAL:O     | 50:D2:10:LEU:C     | 2.58                     | 0.42              |
| 22:DA:1121:C:N3   | 22:DA:1122:G:C8    | 2.88                     | 0.42              |
| 22:DA:1027:A:C5   | 22:DA:1126:A:N3    | 2.88                     | 0.42              |
| 22:DA:1140:C:O4'  | 22:DA:1143:A:C2    | 2.72                     | 0.42              |
| 22:DA:116:C:H4'   | 22:DA:127:A:H5'    | 2.02                     | 0.42              |
| 22:DA:1744:A:C5   | 22:DA:1745:A:C5    | 3.07                     | 0.42              |
| 22:DA:1835:G:C2   | 22:DA:1836:C:C6    | 3.08                     | 0.42              |
| 22:DA:1835:G:N3   | 22:DA:1836:C:C6    | 2.87                     | 0.42              |
| 22:DA:1946:U:H2'  | 22:DA:1947:C:C6    | 2.54                     | 0.42              |
| 22:DA:1973:G:O6   | 22:DA:1974:C:N4    | 2.52                     | 0.42              |
| 22:DA:2038:G:C5   | 22:DA:2039:U:C5    | 3.07                     | 0.42              |
| 22:DA:2056:G:N2   | 22:DA:2057:G:C1'   | 2.83                     | 0.42              |
| 22:DA:2119:A:N1   | 22:DA:2169:A:H2'   | 2.34                     | 0.42              |
| 22:DA:230:G:N3    | 22:DA:231:A:C8     | 2.88                     | 0.42              |
| 22:DA:2366:A:H2'  | 22:DA:2367:G:H5'   | 2.01                     | 0.42              |
| 22:DA:2741:A:C2'  | 22:DA:2742:G:H5'   | 2.49                     | 0.42              |
| 22:DA:2776:A:O4'  | 22:DA:2778:A:C8    | 2.72                     | 0.42              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 22:DA:2836:U:H2'   | 22:DA:2837:A:C8   | 2.54                     | 0.42              |
| 22:DA:308:G:C2     | 22:DA:309:A:N3    | 2.86                     | 0.42              |
| 22:DA:822:G:O6     | 22:DA:943:A:H2    | 2.03                     | 0.42              |
| 24:DC:228:VAL:HG13 | 24:DC:229:ASP:N   | 2.34                     | 0.42              |
| 25:DD:127:PHE:CZ   | 25:DD:160:LYS:HD2 | 2.54                     | 0.42              |
| 25:DD:105:LYS:O    | 25:DD:177:VAL:CG1 | 2.68                     | 0.42              |
| 25:DD:3:GLY:C      | 25:DD:82:PHE:CE1  | 2.93                     | 0.42              |
| 30:DI:19:ASN:OD1   | 30:DI:35:ILE:HG22 | 2.18                     | 0.42              |
| 31:DJ:42:ALA:C     | 31:DJ:44:TYR:H    | 2.23                     | 0.42              |
| 33:DL:120:VAL:CG1  | 33:DL:121:THR:N   | 2.83                     | 0.42              |
| 34:DM:62:LYS:HD3   | 34:DM:64:TRP:CZ2  | 2.55                     | 0.42              |
| 34:DM:67:VAL:CG1   | 34:DM:100:LYS:HD2 | 2.50                     | 0.42              |
| 35:DN:103:ARG:HB2  | 35:DN:110:MET:HE3 | 2.02                     | 0.42              |
| 37:DP:26:VAL:CG1   | 37:DP:28:VAL:HG22 | 2.49                     | 0.42              |
| 37:DP:46:VAL:HG12  | 37:DP:47:VAL:N    | 2.34                     | 0.42              |
| 40:DS:29:VAL:HG22  | 40:DS:71:VAL:HG22 | 2.01                     | 0.42              |
| 1:AA:1241:G:C2     | 1:AA:1242:G:C5    | 3.08                     | 0.42              |
| 1:AA:1521:C:C2     | 1:AA:1522:U:C6    | 3.08                     | 0.42              |
| 1:AA:19:A:C2       | 1:AA:917:G:C4     | 3.07                     | 0.42              |
| 1:AA:223:A:C6      | 1:AA:224:U:O4     | 2.72                     | 0.42              |
| 1:AA:466:A:H5'     | 1:AA:467:U:OP2    | 2.19                     | 0.42              |
| 1:AA:628:G:H2'     | 1:AA:629:A:O4'    | 2.20                     | 0.42              |
| 1:AA:702:A:N6      | 22:BA:1846:G:HO2' | 2.17                     | 0.42              |
| 1:AA:22:G:H4'      | 1:AA:885:G:C8     | 2.55                     | 0.42              |
| 2:AB:118:GLU:O     | 2:AB:121:SER:HB3  | 2.19                     | 0.42              |
| 2:AB:176:ALA:CB    | 2:AB:183:VAL:CG2  | 2.97                     | 0.42              |
| 2:AB:32:PHE:O      | 2:AB:32:PHE:CG    | 2.72                     | 0.42              |
| 4:AD:123:ILE:CD1   | 4:AD:123:ILE:N    | 2.83                     | 0.42              |
| 4:AD:173:VAL:HG13  | 4:AD:174:ASP:N    | 2.34                     | 0.42              |
| 5:AE:72:ILE:CD1    | 5:AE:145:GLU:OE2  | 2.67                     | 0.42              |
| 5:AE:30:ILE:HD11   | 5:AE:54:ARG:NH1   | 2.34                     | 0.42              |
| 8:AH:10:MET:O      | 8:AH:11:LEU:C     | 2.57                     | 0.42              |
| 9:AI:84:THR:HG21   | 9:AI:103:PHE:HB3  | 2.00                     | 0.42              |
| 15:AO:32:LEU:O     | 15:AO:33:THR:C    | 2.58                     | 0.42              |
| 15:AO:85:LEU:HD13  | 15:AO:85:LEU:HA   | 1.83                     | 0.42              |
| 15:AO:87:LEU:HD23  | 15:AO:87:LEU:N    | 2.34                     | 0.42              |
| 18:AR:25:ASP:O     | 18:AR:26:ILE:C    | 2.58                     | 0.42              |
| 49:B1:29:THR:O     | 49:B1:31:PRO:HD2  | 2.20                     | 0.42              |
| 22:BA:1091:G:H2'   | 22:BA:1092:C:C6   | 2.54                     | 0.42              |
| 22:BA:1197:G:H2'   | 22:BA:1198:U:C6   | 2.55                     | 0.42              |
| 22:BA:1449:G:C2    | 22:BA:1450:G:C8   | 3.07                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:BA:1812:U:H2'  | 22:BA:1813:G:H8   | 1.84                     | 0.42              |
| 22:BA:2199:A:N7   | 22:BA:2200:C:C5   | 2.87                     | 0.42              |
| 22:BA:2553:G:C5'  | 22:BA:2554:U:OP2  | 2.67                     | 0.42              |
| 22:BA:2665:A:C2   | 22:BA:2666:C:C2   | 3.08                     | 0.42              |
| 22:BA:278:A:N1    | 22:BA:362:A:C8    | 2.87                     | 0.42              |
| 22:BA:548:G:O2'   | 22:BA:549:G:N1    | 2.52                     | 0.42              |
| 27:BF:92:ARG:CA   | 27:BF:96:MET:HB2  | 2.49                     | 0.42              |
| 29:BH:45:GLU:C    | 29:BH:47:PHE:N    | 2.72                     | 0.42              |
| 33:BL:78:ARG:HG2  | 33:BL:113:ALA:HB3 | 2.02                     | 0.42              |
| 41:BT:40:LYS:HD3  | 41:BT:58:VAL:O    | 2.19                     | 0.42              |
| 45:BX:68:LEU:HD22 | 45:BX:78:TYR:CD1  | 2.55                     | 0.42              |
| 46:BY:9:LYS:O     | 46:BY:12:GLU:HB2  | 2.20                     | 0.42              |
| 1:CA:1300:G:C6    | 1:CA:1335:U:C5    | 3.07                     | 0.42              |
| 1:CA:135:C:O2     | 16:CP:1:MET:CB    | 2.68                     | 0.42              |
| 1:CA:532:A:N6     | 3:CC:192:THR:OG1  | 2.53                     | 0.42              |
| 1:CA:756:C:N3     | 1:CA:757:U:C6     | 2.88                     | 0.42              |
| 2:CB:131:LYS:HE2  | 2:CB:131:LYS:HA   | 2.02                     | 0.42              |
| 2:CB:62:SER:C     | 2:CB:64:LYS:N     | 2.73                     | 0.42              |
| 5:CE:122:ASN:ND2  | 5:CE:123:VAL:N    | 2.68                     | 0.42              |
| 6:CF:18:VAL:HB    | 6:CF:19:PRO:HD3   | 2.01                     | 0.42              |
| 8:CH:104:VAL:HA   | 8:CH:126:ILE:HD12 | 2.01                     | 0.42              |
| 11:CK:126:LYS:O   | 11:CK:127:ARG:CB  | 2.68                     | 0.42              |
| 12:CL:108:LYS:O   | 12:CL:109:ASP:HB2 | 2.20                     | 0.42              |
| 22:DA:117:G:C2    | 22:DA:119:A:N6    | 2.87                     | 0.42              |
| 22:DA:1500:G:C6   | 22:DA:1501:G:N7   | 2.87                     | 0.42              |
| 22:DA:1519:G:H3'  | 22:DA:1520:U:C6   | 2.53                     | 0.42              |
| 22:DA:1603:A:P    | 22:DA:1604:C:OP2  | 2.77                     | 0.42              |
| 22:DA:1310:G:N2   | 22:DA:1605:C:C2   | 2.88                     | 0.42              |
| 22:DA:1793:C:H5'' | 22:DA:1794:A:OP2  | 2.19                     | 0.42              |
| 22:DA:201:C:C5    | 22:DA:202:U:C5    | 3.08                     | 0.42              |
| 22:DA:2233:U:H2'  | 22:DA:2234:G:C8   | 2.54                     | 0.42              |
| 22:DA:2306:C:C5   | 22:DA:2307:G:C8   | 3.08                     | 0.42              |
| 22:DA:2409:G:C6   | 22:DA:2410:G:C6   | 3.07                     | 0.42              |
| 22:DA:2452:C:C4   | 22:DA:2453:A:C6   | 3.07                     | 0.42              |
| 22:DA:2521:C:C2   | 22:DA:2545:G:N2   | 2.88                     | 0.42              |
| 22:DA:2685:G:C4   | 22:DA:2686:G:C8   | 3.07                     | 0.42              |
| 22:DA:2714:G:C5   | 22:DA:2715:C:C5   | 3.07                     | 0.42              |
| 22:DA:282:A:H2'   | 22:DA:283:G:C8    | 2.54                     | 0.42              |
| 22:DA:2879:A:H8   | 22:DA:2881:U:O4   | 2.03                     | 0.42              |
| 22:DA:332:A:HO2'  | 22:DA:334:C:P     | 2.35                     | 0.42              |
| 22:DA:606:U:O2'   | 26:DE:95:LYS:NZ   | 2.52                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:DA:747:U:C4'   | 40:DS:92:ARG:NH1   | 2.82                     | 0.42              |
| 22:DA:770:G:C2    | 22:DA:771:G:C8     | 3.08                     | 0.42              |
| 22:DA:972:A:C6    | 22:DA:973:A:C6     | 3.08                     | 0.42              |
| 25:DD:113:SER:O   | 25:DD:167:ASN:HA   | 2.19                     | 0.42              |
| 30:DI:28:LEU:HD11 | 30:DI:35:ILE:HD12  | 2.01                     | 0.42              |
| 30:DI:24:VAL:CG2  | 30:DI:28:LEU:HD23  | 2.50                     | 0.42              |
| 30:DI:73:THR:HG21 | 30:DI:113:LYS:HE3  | 2.01                     | 0.42              |
| 32:DK:105:ARG:NH1 | 32:DK:122:VAL:O    | 2.53                     | 0.42              |
| 32:DK:62:VAL:HG11 | 32:DK:65:THR:CG2   | 2.48                     | 0.42              |
| 33:DL:29:LYS:C    | 33:DL:30:THR:HG23  | 2.39                     | 0.42              |
| 34:DM:33:LEU:HB2  | 34:DM:117:PHE:CD2  | 2.54                     | 0.42              |
| 35:DN:34:ILE:HD11 | 35:DN:44:LEU:CD2   | 2.50                     | 0.42              |
| 35:DN:87:PHE:O    | 35:DN:88:ALA:C     | 2.58                     | 0.42              |
| 36:DO:74:VAL:HG12 | 36:DO:106:LEU:HD11 | 2.01                     | 0.42              |
| 39:DR:7:SER:O     | 39:DR:9:GLY:N      | 2.47                     | 0.42              |
| 40:DS:59:GLU:HG2  | 40:DS:64:ALA:HA    | 2.01                     | 0.42              |
| 45:DX:65:ASP:O    | 45:DX:66:THR:C     | 2.57                     | 0.42              |
| 1:AA:1277:C:O2'   | 1:AA:1279:G:H8     | 1.99                     | 0.42              |
| 1:AA:1317:C:H2'   | 1:AA:1318:A:H5'    | 2.02                     | 0.42              |
| 1:AA:251:G:H4'    | 1:AA:252:U:O5'     | 2.20                     | 0.42              |
| 1:AA:340:U:N3     | 1:AA:341:C:C5      | 2.88                     | 0.42              |
| 1:AA:363:A:O2'    | 1:AA:364:A:H5'     | 2.18                     | 0.42              |
| 1:AA:575:G:C6     | 1:AA:821:G:C8      | 3.07                     | 0.42              |
| 1:AA:651:C:H2'    | 1:AA:652:U:O5'     | 2.20                     | 0.42              |
| 1:AA:764:C:C2'    | 1:AA:765:G:H5'     | 2.49                     | 0.42              |
| 2:AB:35:ARG:HB3   | 2:AB:40:ILE:HD11   | 1.99                     | 0.42              |
| 3:AC:47:LEU:HB3   | 3:AC:50:ALA:HB3    | 2.00                     | 0.42              |
| 8:AH:7:ILE:O      | 8:AH:11:LEU:HG     | 2.20                     | 0.42              |
| 9:AI:63:LEU:CD2   | 9:AI:63:LEU:N      | 2.82                     | 0.42              |
| 10:AJ:34:ALA:O    | 10:AJ:35:GLN:HB3   | 2.19                     | 0.42              |
| 11:AK:55:SER:O    | 11:AK:57:LYS:N     | 2.52                     | 0.42              |
| 12:AL:18:LYS:HG3  | 12:AL:18:LYS:O     | 2.19                     | 0.42              |
| 12:AL:21:VAL:O    | 12:AL:21:VAL:HG13  | 2.20                     | 0.42              |
| 16:AP:76:LYS:O    | 16:AP:76:LYS:HG3   | 2.20                     | 0.42              |
| 19:AS:15:LEU:CD1  | 19:AS:33:THR:HG21  | 2.50                     | 0.42              |
| 40:BS:19:LEU:HB3  | 48:B0:22:LEU:HD11  | 2.02                     | 0.42              |
| 22:BA:2015:A:C6   | 48:B0:3:VAL:HG23   | 2.54                     | 0.42              |
| 22:BA:1177:G:H2'  | 22:BA:1178:C:O4'   | 2.20                     | 0.42              |
| 22:BA:1564:C:O2'  | 22:BA:1565:C:H5'   | 2.20                     | 0.42              |
| 22:BA:1730:C:H4'  | 22:BA:1730:C:OP1   | 2.19                     | 0.42              |
| 22:BA:2020:A:H5'  | 48:B0:9:THR:HG22   | 2.01                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:BA:2208:C:O2'  | 22:BA:2209:G:H5'  | 2.20                     | 0.42              |
| 22:BA:2236:U:H2'  | 22:BA:2237:G:O4'  | 2.20                     | 0.42              |
| 22:BA:2394:C:P    | 51:B3:30:ARG:HH21 | 2.43                     | 0.42              |
| 22:BA:2660:A:H2'  | 22:BA:2661:G:O4'  | 2.18                     | 0.42              |
| 22:BA:26:G:H1'    | 22:BA:514:A:H61   | 1.83                     | 0.42              |
| 22:BA:301:G:H1'   | 22:BA:302:C:C6    | 2.55                     | 0.42              |
| 22:BA:773:U:H5'   | 24:BC:47:GLY:HA3  | 2.01                     | 0.42              |
| 22:BA:998:C:P     | 38:BQ:92:ARG:NH2  | 2.92                     | 0.42              |
| 23:BB:90:C:H2'    | 23:BB:91:C:O4'    | 2.20                     | 0.42              |
| 23:BB:97:C:H2'    | 23:BB:98:G:H5'    | 2.02                     | 0.42              |
| 24:BC:7:LYS:HB3   | 24:BC:8:PRO:HD2   | 2.02                     | 0.42              |
| 26:BE:54:GLY:O    | 26:BE:74:LYS:HE2  | 2.20                     | 0.42              |
| 27:BF:158:THR:CG2 | 27:BF:160:ALA:CB  | 2.98                     | 0.42              |
| 27:BF:119:ALA:HB2 | 27:BF:177:PHE:CD2 | 2.54                     | 0.42              |
| 29:BH:114:GLU:CB  | 29:BH:133:GLN:O   | 2.66                     | 0.42              |
| 31:BJ:38:GLY:O    | 31:BJ:44:TYR:HB2  | 2.20                     | 0.42              |
| 31:BJ:64:VAL:HG11 | 31:BJ:68:LYS:HB2  | 2.01                     | 0.42              |
| 36:BO:28:VAL:CG2  | 36:BO:29:HIS:N    | 2.83                     | 0.42              |
| 1:CA:1036:A:H3'   | 1:CA:1037:C:C6    | 2.54                     | 0.42              |
| 1:CA:1139:G:O6    | 1:CA:1143:G:N2    | 2.52                     | 0.42              |
| 1:CA:1175:G:O6    | 1:CA:1182:G:O6    | 2.37                     | 0.42              |
| 1:CA:1349:A:OP1   | 9:CI:123:ARG:N    | 2.52                     | 0.42              |
| 1:CA:411:A:C6     | 1:CA:429:U:C4     | 3.07                     | 0.42              |
| 1:CA:41:G:H2'     | 1:CA:42:G:C8      | 2.55                     | 0.42              |
| 1:CA:445:G:C2     | 1:CA:490:C:C2     | 3.07                     | 0.42              |
| 1:CA:689:C:H2'    | 1:CA:690:G:O4'    | 2.19                     | 0.42              |
| 1:CA:72:A:N6      | 1:CA:73:C:H42     | 2.18                     | 0.42              |
| 1:CA:833:G:O2'    | 1:CA:834:U:H5'    | 2.19                     | 0.42              |
| 1:CA:899:C:OP1    | 1:CA:899:C:H6     | 2.02                     | 0.42              |
| 4:CD:198:HIS:CE1  | 4:CD:199:LEU:CD2  | 3.03                     | 0.42              |
| 4:CD:53:VAL:CG2   | 4:CD:54:GLN:N     | 2.82                     | 0.42              |
| 4:CD:4:TYR:CZ     | 4:CD:6:GLY:HA3    | 2.54                     | 0.42              |
| 5:CE:122:ASN:ND2  | 5:CE:123:VAL:H    | 2.17                     | 0.42              |
| 5:CE:57:PRO:O     | 5:CE:60:ILE:HG13  | 2.18                     | 0.42              |
| 6:CF:64:VAL:HG12  | 6:CF:65:GLU:H     | 1.85                     | 0.42              |
| 9:CI:130:ARG:HA   | 9:CI:130:ARG:HD2  | 1.82                     | 0.42              |
| 13:CM:45:ILE:O    | 13:CM:45:ILE:HG22 | 2.20                     | 0.42              |
| 6:CF:86:ARG:HD3   | 18:CR:64:TYR:CE1  | 2.54                     | 0.42              |
| 14:CN:46:LEU:HD23 | 19:CS:10:PHE:HB2  | 2.02                     | 0.42              |
| 21:CU:14:VAL:O    | 21:CU:16:LEU:CG   | 2.66                     | 0.42              |
| 49:D1:19:HIS:CD2  | 49:D1:49:TYR:OH   | 2.72                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:DA:1869:G:C2   | 22:DA:1873:G:C6    | 3.07                     | 0.42              |
| 22:DA:2322:A:C5   | 22:DA:2323:G:C5    | 3.07                     | 0.42              |
| 22:DA:2446:G:H3'  | 22:DA:2447:G:H5''  | 2.01                     | 0.42              |
| 22:DA:2560:A:H2'  | 22:DA:2561:U:O4'   | 2.19                     | 0.42              |
| 22:DA:2702:G:N7   | 22:DA:2703:C:C5    | 2.87                     | 0.42              |
| 22:DA:2736:A:C2   | 22:DA:2737:G:C8    | 3.08                     | 0.42              |
| 22:DA:2861:U:C2   | 22:DA:2862:G:C8    | 3.07                     | 0.42              |
| 22:DA:503:A:N6    | 22:DA:505:A:N6     | 2.67                     | 0.42              |
| 22:DA:618:G:N2    | 22:DA:619:G:H1'    | 2.35                     | 0.42              |
| 22:DA:790:U:C4    | 22:DA:794:A:O2'    | 2.73                     | 0.42              |
| 22:DA:864:G:C6    | 22:DA:865:C:C4     | 3.07                     | 0.42              |
| 22:DA:87:U:O2     | 46:DY:44:LYS:NZ    | 2.48                     | 0.42              |
| 24:DC:166:ALA:HB3 | 24:DC:173:THR:HB   | 1.99                     | 0.42              |
| 27:DF:122:PHE:CE1 | 27:DF:166:GLY:CA   | 3.02                     | 0.42              |
| 22:DA:2305:U:O4'  | 27:DF:131:GLY:HA3  | 2.18                     | 0.42              |
| 27:DF:77:PHE:C    | 27:DF:78:LYS:HG3   | 2.40                     | 0.42              |
| 29:DH:69:ALA:HB2  | 29:DH:138:VAL:HG12 | 2.02                     | 0.42              |
| 35:DN:52:ILE:HD12 | 35:DN:94:TYR:HB2   | 2.02                     | 0.42              |
| 36:DO:88:LYS:HA   | 36:DO:88:LYS:HE3   | 2.02                     | 0.42              |
| 41:DT:65:GLY:O    | 41:DT:66:LYS:C     | 2.57                     | 0.42              |
| 42:DU:13:VAL:CG2  | 42:DU:39:ILE:HG21  | 2.50                     | 0.42              |
| 1:AA:1033:G:O2'   | 1:AA:1034:G:H5'    | 2.19                     | 0.42              |
| 1:AA:1100:C:O2'   | 1:AA:1102:A:OP1    | 2.32                     | 0.42              |
| 1:AA:1151:A:C4    | 1:AA:1152:A:C8     | 3.08                     | 0.42              |
| 1:AA:19:A:H1'     | 1:AA:917:G:N2      | 2.34                     | 0.42              |
| 1:AA:244:U:O4     | 1:AA:906:A:H1'     | 2.19                     | 0.42              |
| 1:AA:350:G:O2'    | 1:AA:351:G:H5'     | 2.20                     | 0.42              |
| 1:AA:616:G:C2'    | 1:AA:617:G:H5'     | 2.50                     | 0.42              |
| 1:AA:596:A:N6     | 1:AA:645:G:N1      | 2.68                     | 0.42              |
| 1:AA:844:G:H2'    | 1:AA:845:A:H5''    | 2.02                     | 0.42              |
| 2:AB:148:LEU:HD22 | 2:AB:148:LEU:HA    | 1.92                     | 0.42              |
| 2:AB:186:ILE:HD11 | 2:AB:204:ASP:CB    | 2.50                     | 0.42              |
| 9:AI:30:ILE:CG2   | 9:AI:65:ILE:HD11   | 2.50                     | 0.42              |
| 9:AI:6:TYR:HB2    | 9:AI:89:GLU:OE2    | 2.19                     | 0.42              |
| 10:AJ:87:LEU:HD13 | 10:AJ:88:MET:N     | 2.34                     | 0.42              |
| 10:AJ:86:ALA:O    | 10:AJ:90:LEU:HB2   | 2.20                     | 0.42              |
| 11:AK:102:ALA:C   | 11:AK:104:GLY:N    | 2.73                     | 0.42              |
| 11:AK:52:PHE:O    | 11:AK:57:LYS:HB3   | 2.20                     | 0.42              |
| 15:AO:87:LEU:O    | 15:AO:88:ARG:HB2   | 2.19                     | 0.42              |
| 49:B1:25:LYS:HE3  | 49:B1:30:LYS:O     | 2.20                     | 0.42              |
| 51:B3:7:VAL:HB    | 51:B3:61:CYS:HB3   | 2.00                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:BA:1299:G:H8    | 22:BA:1299:G:O5'   | 2.03                     | 0.42              |
| 22:BA:1366:A:C6    | 22:BA:1367:A:C4    | 3.08                     | 0.42              |
| 22:BA:136:G:O5'    | 22:BA:136:G:H8     | 2.03                     | 0.42              |
| 22:BA:1539:U:H2'   | 22:BA:1540:G:C8    | 2.53                     | 0.42              |
| 22:BA:158:U:O2     | 22:BA:158:U:H2'    | 2.18                     | 0.42              |
| 22:BA:1927:A:H2'   | 22:BA:1928:A:C8    | 2.54                     | 0.42              |
| 22:BA:2727:A:H2'   | 22:BA:2728:U:H5'   | 2.01                     | 0.42              |
| 22:BA:2805:C:C4    | 22:BA:2806:C:C4    | 3.07                     | 0.42              |
| 22:BA:451:U:C2     | 22:BA:453:A:N7     | 2.88                     | 0.42              |
| 22:BA:637:A:OP1    | 33:BL:130:GLY:HA3  | 2.20                     | 0.42              |
| 22:BA:80:G:N2      | 22:BA:81:G:H1'     | 2.35                     | 0.42              |
| 22:BA:875:G:C2'    | 22:BA:876:C:H5'    | 2.49                     | 0.42              |
| 22:BA:959:A:N1     | 22:BA:960:A:C2     | 2.87                     | 0.42              |
| 27:BF:108:VAL:HG13 | 27:BF:114:PHE:CZ   | 2.54                     | 0.42              |
| 29:BH:116:ARG:HB3  | 29:BH:131:SER:O    | 2.20                     | 0.42              |
| 29:BH:118:PRO:O    | 29:BH:119:ASN:CB   | 2.68                     | 0.42              |
| 29:BH:89:LYS:O     | 29:BH:90:LEU:C     | 2.58                     | 0.42              |
| 30:BI:101:ILE:HD11 | 30:BI:138:LEU:HD13 | 2.01                     | 0.42              |
| 30:BI:101:ILE:HG22 | 30:BI:102:SER:N    | 2.35                     | 0.42              |
| 31:BJ:70:THR:OG1   | 31:BJ:71:ASP:OD2   | 2.35                     | 0.42              |
| 34:BM:68:PHE:CD2   | 34:BM:68:PHE:C     | 2.93                     | 0.42              |
| 34:BM:4:PRO:HB2    | 34:BM:7:THR:CG2    | 2.49                     | 0.42              |
| 37:BP:53:ARG:HG3   | 37:BP:53:ARG:HH11  | 1.82                     | 0.42              |
| 41:BT:2:ILE:HA     | 41:BT:3:ARG:CB     | 2.47                     | 0.42              |
| 41:BT:71:GLY:O     | 41:BT:73:ARG:N     | 2.52                     | 0.42              |
| 1:CA:1261:A:C6     | 1:CA:1275:A:C4     | 3.08                     | 0.42              |
| 1:CA:1286:U:H2'    | 1:CA:1286:U:O2     | 2.18                     | 0.42              |
| 1:CA:210:C:OP1     | 1:CA:211:G:OP1     | 2.37                     | 0.42              |
| 1:CA:408:A:H2'     | 1:CA:409:U:O4'     | 2.19                     | 0.42              |
| 1:CA:509:A:N3      | 1:CA:543:U:O2'     | 2.46                     | 0.42              |
| 1:CA:599:C:H4'     | 8:CH:122:GLY:C     | 2.40                     | 0.42              |
| 1:CA:609:A:C5      | 1:CA:610:U:C6      | 3.07                     | 0.42              |
| 1:CA:927:G:OP2     | 1:CA:927:G:H4'     | 2.20                     | 0.42              |
| 1:CA:994:A:C2      | 1:CA:995:C:C1'     | 3.02                     | 0.42              |
| 2:CB:71:GLY:HA3    | 2:CB:164:ILE:CG2   | 2.50                     | 0.42              |
| 2:CB:217:VAL:O     | 2:CB:220:THR:HG22  | 2.20                     | 0.42              |
| 3:CC:179:ARG:HD2   | 3:CC:179:ARG:C     | 2.40                     | 0.42              |
| 3:CC:75:ILE:O      | 3:CC:75:ILE:CG1    | 2.68                     | 0.42              |
| 5:CE:126:LYS:HA    | 5:CE:126:LYS:CE    | 2.49                     | 0.42              |
| 7:CG:43:VAL:HG12   | 7:CG:44:TYR:CD1    | 2.55                     | 0.42              |
| 1:CA:1377:A:C4     | 7:CG:7:ILE:HD11    | 2.54                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:1291:U:H4'    | 9:CI:42:GLU:HG2    | 2.01                     | 0.42              |
| 11:CK:15:GLN:OE1   | 11:CK:17:SER:N     | 2.53                     | 0.42              |
| 11:CK:77:TYR:O     | 11:CK:78:GLY:C     | 2.58                     | 0.42              |
| 12:CL:110:ARG:NE   | 12:CL:117:TYR:CD2  | 2.88                     | 0.42              |
| 13:CM:14:HIS:HB2   | 13:CM:17:ILE:HD12  | 2.01                     | 0.42              |
| 22:DA:84:A:C2      | 22:DA:103:A:C5     | 3.08                     | 0.42              |
| 22:DA:941:A:O2'    | 22:DA:1190:G:O3'   | 2.37                     | 0.42              |
| 22:DA:1263:U:C4'   | 48:D0:7:LYS:HE3    | 2.49                     | 0.42              |
| 22:DA:1262:A:N1    | 22:DA:1263:U:O2    | 2.52                     | 0.42              |
| 22:DA:1562:U:C4    | 22:DA:1563:U:C4    | 3.07                     | 0.42              |
| 22:DA:1714:U:O5'   | 22:DA:1715:G:H5'   | 2.19                     | 0.42              |
| 22:DA:1838:C:H4'   | 22:DA:1839:G:H8    | 1.85                     | 0.42              |
| 22:DA:1663:G:C6    | 22:DA:1992:G:C8    | 3.08                     | 0.42              |
| 22:DA:563:A:C6     | 22:DA:2018:G:C4    | 3.08                     | 0.42              |
| 22:DA:2057:G:P     | 57:DA:3665:HOH:O   | 2.77                     | 0.42              |
| 22:DA:233:A:C2     | 22:DA:234:U:H1'    | 2.54                     | 0.42              |
| 22:DA:2371:G:C2    | 22:DA:2372:U:C5    | 3.07                     | 0.42              |
| 22:DA:2461:A:H1'   | 22:DA:2492:U:N3    | 2.35                     | 0.42              |
| 22:DA:2718:G:O2'   | 37:DP:96:LYS:HG3   | 2.20                     | 0.42              |
| 22:DA:2735:G:H2'   | 22:DA:2736:A:H8    | 1.84                     | 0.42              |
| 22:DA:572:A:H5''   | 22:DA:573:U:OP2    | 2.19                     | 0.42              |
| 22:DA:656:G:O2'    | 22:DA:657:U:H5'    | 2.20                     | 0.42              |
| 22:DA:717:C:N4     | 22:DA:718:A:C2     | 2.87                     | 0.42              |
| 22:DA:77:G:H2'     | 22:DA:78:U:O4'     | 2.19                     | 0.42              |
| 22:DA:7:G:HO2'     | 31:DJ:15:TRP:HZ2   | 1.64                     | 0.42              |
| 23:DB:68:C:H2'     | 23:DB:69:G:O4'     | 2.19                     | 0.42              |
| 24:DC:130:LEU:HD11 | 24:DC:135:ILE:HG12 | 2.02                     | 0.42              |
| 22:DA:1824:G:O3'   | 24:DC:247:PRO:CD   | 2.67                     | 0.42              |
| 24:DC:82:GLU:OE1   | 24:DC:103:TYR:OH   | 2.31                     | 0.42              |
| 25:DD:187:LEU:HD21 | 25:DD:203:VAL:HG11 | 2.01                     | 0.42              |
| 26:DE:129:PRO:HG3  | 26:DE:156:ASN:OD1  | 2.20                     | 0.42              |
| 22:DA:660:C:H5''   | 26:DE:94:GLN:OE1   | 2.20                     | 0.42              |
| 27:DF:117:LEU:O    | 27:DF:118:SER:C    | 2.57                     | 0.42              |
| 27:DF:174:ASP:O    | 27:DF:175:PHE:O    | 2.37                     | 0.42              |
| 28:DG:155:GLU:OE1  | 28:DG:158:LYS:HG3  | 2.20                     | 0.42              |
| 29:DH:41:LYS:HE2   | 29:DH:44:ILE:CD1   | 2.50                     | 0.42              |
| 29:DH:72:ILE:O     | 29:DH:72:ILE:CG2   | 2.67                     | 0.42              |
| 31:DJ:6:ALA:O      | 31:DJ:7:LYS:CB     | 2.68                     | 0.42              |
| 34:DM:22:GLN:O     | 34:DM:24:THR:N     | 2.53                     | 0.42              |
| 35:DN:108:ALA:HB3  | 35:DN:110:MET:HE3  | 2.02                     | 0.42              |
| 40:DS:76:VAL:HG13  | 40:DS:103:ILE:HG12 | 2.02                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 41:DT:39:THR:HG23 | 41:DT:42:GLU:HB2  | 2.02                     | 0.42              |
| 22:DA:927:A:C2    | 47:DZ:43:ALA:HB1  | 2.55                     | 0.42              |
| 1:AA:102:G:C2     | 1:AA:103:U:C6     | 3.08                     | 0.42              |
| 1:AA:1053:G:C6    | 1:AA:1199:U:C2    | 3.07                     | 0.42              |
| 1:AA:1217:C:H2'   | 1:AA:1218:C:H6    | 1.83                     | 0.42              |
| 1:AA:21:G:H2'     | 1:AA:22:G:C8      | 2.55                     | 0.42              |
| 1:AA:443:C:C2     | 1:AA:444:G:C8     | 3.07                     | 0.42              |
| 1:AA:53:A:H2'     | 1:AA:54:C:O5'     | 2.20                     | 0.42              |
| 1:AA:714:G:O2'    | 1:AA:715:A:H5'    | 2.19                     | 0.42              |
| 1:AA:721:G:H4'    | 1:AA:722:G:C5'    | 2.50                     | 0.42              |
| 1:AA:958:A:N1     | 19:AS:54:GLY:HA3  | 2.34                     | 0.42              |
| 2:AB:151:ILE:O    | 2:AB:153:ASP:N    | 2.53                     | 0.42              |
| 2:AB:19:GLN:O     | 2:AB:38:VAL:HG23  | 2.19                     | 0.42              |
| 3:AC:120:ILE:O    | 3:AC:124:LEU:HG   | 2.20                     | 0.42              |
| 5:AE:133:PRO:HA   | 5:AE:136:VAL:CG1  | 2.49                     | 0.42              |
| 9:AI:91:ASP:C     | 9:AI:91:ASP:OD2   | 2.58                     | 0.42              |
| 1:AA:1152:A:H5'   | 10:AJ:15:HIS:CD2  | 2.55                     | 0.42              |
| 12:AL:55:VAL:HG21 | 12:AL:80:ILE:HD11 | 2.00                     | 0.42              |
| 15:AO:2:SER:O     | 15:AO:3:LEU:HB2   | 2.19                     | 0.42              |
| 16:AP:78:VAL:O    | 16:AP:79:ASN:HB2  | 2.20                     | 0.42              |
| 18:AR:55:LEU:HD22 | 18:AR:55:LEU:HA   | 1.91                     | 0.42              |
| 22:BA:1735:A:C2'  | 22:BA:1736:U:H5'  | 2.50                     | 0.42              |
| 22:BA:2076:U:C5'  | 22:BA:2076:U:O2   | 2.68                     | 0.42              |
| 22:BA:275:C:H3'   | 22:BA:276:U:H5''  | 2.01                     | 0.42              |
| 22:BA:2884:U:O4'  | 22:BA:2884:U:O2   | 2.37                     | 0.42              |
| 22:BA:971:G:OP2   | 22:BA:974:G:N2    | 2.53                     | 0.42              |
| 24:BC:125:LYS:CG  | 24:BC:128:ASN:ND2 | 2.83                     | 0.42              |
| 24:BC:197:ASN:O   | 24:BC:197:ASN:CG  | 2.57                     | 0.42              |
| 30:BI:96:ASP:OD1  | 30:BI:97:LYS:N    | 2.53                     | 0.42              |
| 33:BL:53:GLY:O    | 33:BL:54:GLN:C    | 2.58                     | 0.42              |
| 38:BQ:19:LYS:O    | 38:BQ:22:LYS:HG3  | 2.20                     | 0.42              |
| 41:BT:50:LEU:CD1  | 41:BT:50:LEU:N    | 2.83                     | 0.42              |
| 42:BU:41:LEU:HD13 | 42:BU:60:GLU:OE2  | 2.20                     | 0.42              |
| 46:BY:32:ALA:HB2  | 46:BY:37:LEU:CD2  | 2.50                     | 0.42              |
| 1:CA:1130:A:C8    | 1:CA:1146:A:N1    | 2.88                     | 0.42              |
| 1:CA:1132:C:H2'   | 1:CA:1133:G:C1'   | 2.50                     | 0.42              |
| 1:CA:1269:A:H1'   | 1:CA:1326:U:H1'   | 2.02                     | 0.42              |
| 1:CA:155:A:C2     | 1:CA:167:A:C4     | 3.08                     | 0.42              |
| 1:CA:337:G:H2'    | 1:CA:338:A:C8     | 2.55                     | 0.42              |
| 1:CA:409:U:C4     | 1:CA:410:G:C5     | 3.08                     | 0.42              |
| 1:CA:728:A:C2     | 1:CA:729:A:C4     | 3.08                     | 0.42              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 4:CD:119:SER:O    | 4:CD:131:ASN:OD1  | 2.38                     | 0.42              |
| 4:CD:169:THR:HG22 | 4:CD:184:ARG:NH2  | 2.34                     | 0.42              |
| 4:CD:59:GLN:CA    | 4:CD:59:GLN:OE1   | 2.64                     | 0.42              |
| 5:CE:157:ARG:C    | 5:CE:159:LYS:N    | 2.72                     | 0.42              |
| 6:CF:12:PRO:O     | 6:CF:15:SER:OG    | 2.23                     | 0.42              |
| 7:CG:4:ARG:HG3    | 7:CG:5:ARG:N      | 2.35                     | 0.42              |
| 18:CR:42:SER:HB2  | 18:CR:46:GLY:O    | 2.19                     | 0.42              |
| 19:CS:44:MET:CB   | 19:CS:62:VAL:HG11 | 2.50                     | 0.42              |
| 51:D3:7:VAL:O     | 51:D3:10:ALA:HB3  | 2.19                     | 0.42              |
| 22:DA:1047:G:H4'  | 22:DA:1048:A:H5'  | 2.02                     | 0.42              |
| 22:DA:1190:G:OP1  | 33:DL:32:GLY:CA   | 2.68                     | 0.42              |
| 22:DA:1598:A:C6   | 22:DA:1599:U:N3   | 2.88                     | 0.42              |
| 22:DA:161:A:P     | 22:DA:162:U:H3'   | 2.60                     | 0.42              |
| 22:DA:1654:A:N7   | 22:DA:2005:A:C2   | 2.88                     | 0.42              |
| 22:DA:120:U:O4    | 22:DA:177:G:C8    | 2.73                     | 0.42              |
| 22:DA:1802:A:C2   | 22:DA:1803:A:N3   | 2.88                     | 0.42              |
| 22:DA:2166:U:H2'  | 22:DA:2167:U:H5'  | 2.02                     | 0.42              |
| 22:DA:2186:G:C5   | 22:DA:2187:U:C4   | 3.08                     | 0.42              |
| 22:DA:2216:G:H2'  | 22:DA:2217:G:H8   | 1.83                     | 0.42              |
| 22:DA:2320:U:H4'  | 22:DA:2321:U:C6   | 2.55                     | 0.42              |
| 22:DA:2360:G:H1'  | 33:DL:60:ARG:CD   | 2.49                     | 0.42              |
| 22:DA:2663:G:H3'  | 22:DA:2664:G:C8   | 2.54                     | 0.42              |
| 22:DA:2734:A:N7   | 22:DA:2735:G:C8   | 2.88                     | 0.42              |
| 22:DA:295:G:N2    | 22:DA:296:U:C6    | 2.88                     | 0.42              |
| 22:DA:83:A:H4'    | 22:DA:83:A:OP1    | 2.19                     | 0.42              |
| 26:DE:91:ASP:O    | 26:DE:91:ASP:CG   | 2.58                     | 0.42              |
| 27:DF:128:TYR:CB  | 27:DF:170:LEU:CD1 | 2.98                     | 0.42              |
| 28:DG:144:VAL:O   | 28:DG:144:VAL:CG1 | 2.68                     | 0.42              |
| 29:DH:127:GLU:HA  | 29:DH:144:VAL:O   | 2.19                     | 0.42              |
| 29:DH:31:VAL:HG12 | 29:DH:32:PRO:HD3  | 2.02                     | 0.42              |
| 22:DA:1082:U:OP1  | 30:DI:124:ALA:HB2 | 2.19                     | 0.42              |
| 33:DL:86:GLU:HG3  | 33:DL:86:GLU:O    | 2.19                     | 0.42              |
| 35:DN:24:MET:HE3  | 35:DN:44:LEU:HB2  | 2.02                     | 0.42              |
| 35:DN:33:ILE:HD12 | 35:DN:118:ARG:NH1 | 2.34                     | 0.42              |
| 35:DN:46:ARG:O    | 35:DN:50:PRO:HG2  | 2.20                     | 0.42              |
| 23:DB:7:G:C5'     | 36:DO:29:HIS:CE1  | 3.01                     | 0.42              |
| 38:DQ:47:TYR:HD1  | 39:DR:74:ILE:HG23 | 1.84                     | 0.42              |
| 38:DQ:58:ARG:NH2  | 38:DQ:92:ARG:NH1  | 2.68                     | 0.42              |
| 39:DR:66:HIS:CD2  | 39:DR:94:THR:HG23 | 2.55                     | 0.42              |
| 57:DB:307:HOH:O   | 43:DV:14:LYS:CE   | 2.68                     | 0.42              |
| 1:AA:1118:U:O2    | 1:AA:1179:A:C6    | 2.73                     | 0.42              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:AA:200:G:N2    | 1:AA:218:U:O2     | 2.52                     | 0.42              |
| 1:AA:198:G:C5    | 1:AA:220:G:C2     | 3.08                     | 0.42              |
| 1:AA:596:A:C5    | 1:AA:645:G:C2     | 3.08                     | 0.42              |
| 2:AB:14:VAL:HG23 | 2:AB:208:ARG:NH2  | 2.35                     | 0.42              |
| 3:AC:152:GLU:HA  | 3:AC:167:TRP:HA   | 2.02                     | 0.42              |
| 3:AC:37:PHE:O    | 3:AC:41:GLN:HB2   | 2.20                     | 0.42              |
| 3:AC:42:TYR:CZ   | 3:AC:46:GLU:HG3   | 2.54                     | 0.42              |
| 6:AF:91:ARG:HG2  | 6:AF:93:LYS:HD3   | 2.01                     | 0.42              |
| 6:AF:92:THR:HG22 | 6:AF:93:LYS:N     | 2.34                     | 0.42              |
| 8:AH:105:SER:HB2 | 8:AH:126:ILE:HD11 | 2.01                     | 0.42              |
| 8:AH:10:MET:C    | 8:AH:12:THR:N     | 2.73                     | 0.42              |
| 10:AJ:61:ALA:O   | 10:AJ:62:ARG:HB2  | 2.18                     | 0.42              |
| 12:AL:60:GLY:O   | 12:AL:61:PHE:C    | 2.58                     | 0.42              |
| 19:AS:29:LYS:HG2 | 19:AS:30:PRO:HD2  | 2.02                     | 0.42              |
| 22:BA:83:A:C6    | 22:BA:101:A:C4    | 3.08                     | 0.42              |
| 22:BA:1046:A:H4' | 22:BA:1046:A:OP2  | 2.19                     | 0.42              |
| 22:BA:1495:A:O2' | 22:BA:1496:A:H5'  | 2.20                     | 0.42              |
| 22:BA:1745:A:C2  | 22:BA:1746:A:C8   | 3.08                     | 0.42              |
| 22:BA:184:C:H2'  | 22:BA:185:G:H8    | 1.85                     | 0.42              |
| 22:BA:1131:G:O2' | 22:BA:2026:U:H5'  | 2.20                     | 0.42              |
| 22:BA:2151:U:H2' | 22:BA:2152:G:N7   | 2.35                     | 0.42              |
| 22:BA:2193:G:C2' | 22:BA:2194:U:H5'  | 2.49                     | 0.42              |
| 22:BA:2218:G:O2' | 22:BA:2219:U:H5'  | 2.19                     | 0.42              |
| 22:BA:2489:U:O2  | 22:BA:2491:U:C4   | 2.72                     | 0.42              |
| 22:BA:503:A:H4'  | 22:BA:504:A:O5'   | 2.19                     | 0.42              |
| 22:BA:622:G:H5'' | 57:BA:3294:HOH:O  | 2.20                     | 0.42              |
| 23:BB:60:C:N4    | 57:BB:303:HOH:O   | 2.52                     | 0.42              |
| 26:BE:29:HIS:O   | 26:BE:33:VAL:HG23 | 2.20                     | 0.42              |
| 27:BF:27:GLN:O   | 27:BF:29:PRO:HD3  | 2.20                     | 0.42              |
| 28:BG:35:ARG:HD3 | 28:BG:71:LEU:HD13 | 2.01                     | 0.42              |
| 29:BH:82:SER:HG  | 29:BH:90:LEU:HG   | 1.85                     | 0.42              |
| 30:BI:131:GLY:O  | 30:BI:135:SER:N   | 2.53                     | 0.42              |
| 33:BL:85:VAL:HB  | 33:BL:94:THR:HG23 | 2.01                     | 0.42              |
| 22:BA:1454:C:H5' | 35:BN:63:ARG:CD   | 2.49                     | 0.42              |
| 1:CA:1070:U:O2   | 1:CA:1071:C:C6    | 2.73                     | 0.42              |
| 1:CA:1130:A:N9   | 1:CA:1146:A:C2    | 2.87                     | 0.42              |
| 1:CA:1530:G:H2'  | 1:CA:1531:A:C8    | 2.54                     | 0.42              |
| 1:CA:345:C:OP1   | 37:DP:39:ARG:HD3  | 2.20                     | 0.42              |
| 1:CA:373:A:N3    | 1:CA:374:A:C8     | 2.88                     | 0.42              |
| 1:CA:780:A:N3    | 1:CA:803:G:C2     | 2.88                     | 0.42              |
| 2:CB:30:PHE:CD1  | 2:CB:30:PHE:N     | 2.85                     | 0.42              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 2:CB:82:ASP:N      | 2:CB:85:LEU:HB3   | 2.35                     | 0.42              |
| 10:CJ:73:LEU:HD23  | 10:CJ:73:LEU:C    | 2.40                     | 0.42              |
| 18:CR:45:THR:OG1   | 18:CR:47:THR:HG23 | 2.20                     | 0.42              |
| 6:CF:59:TYR:CE2    | 18:CR:67:LEU:CD2  | 3.03                     | 0.42              |
| 1:CA:1221:G:O3'    | 19:CS:77:THR:HB   | 2.20                     | 0.42              |
| 20:CT:79:LEU:O     | 20:CT:83:ILE:HG23 | 2.20                     | 0.42              |
| 49:D1:26:ASN:O     | 49:D1:27:LYS:C    | 2.58                     | 0.42              |
| 22:DA:1126:A:H4'   | 22:DA:1127:A:O5'  | 2.20                     | 0.42              |
| 22:DA:1355:G:C6    | 22:DA:1356:G:C8   | 3.08                     | 0.42              |
| 22:DA:1461:C:N3    | 22:DA:1462:C:C5   | 2.88                     | 0.42              |
| 22:DA:1340:U:H5    | 22:DA:1603:A:C8   | 2.34                     | 0.42              |
| 22:DA:1874:C:C5'   | 22:DA:1875:G:OP2  | 2.68                     | 0.42              |
| 22:DA:2005:A:H5''  | 57:DA:3382:HOH:O  | 2.19                     | 0.42              |
| 22:DA:2118:U:O4    | 22:DA:2149:U:C1'  | 2.68                     | 0.42              |
| 22:DA:2191:A:C6    | 22:DA:2192:U:C4   | 3.07                     | 0.42              |
| 22:DA:966:G:H4'    | 22:DA:2272:U:O2   | 2.19                     | 0.42              |
| 22:DA:2276:G:O2'   | 22:DA:2277:G:H5'  | 2.19                     | 0.42              |
| 22:DA:2283:C:H2'   | 22:DA:2284:A:H5'  | 2.02                     | 0.42              |
| 22:DA:2330:G:C2    | 22:DA:2386:A:C2   | 3.08                     | 0.42              |
| 22:DA:2371:G:C2    | 22:DA:2372:U:C6   | 3.07                     | 0.42              |
| 22:DA:300:A:O2'    | 22:DA:318:C:O2'   | 2.08                     | 0.42              |
| 22:DA:303:G:C6     | 22:DA:304:U:C4    | 3.08                     | 0.42              |
| 22:DA:324:A:H2'    | 22:DA:325:G:O4'   | 2.20                     | 0.42              |
| 22:DA:681:G:C6     | 22:DA:682:G:N7    | 2.88                     | 0.42              |
| 22:DA:728:G:HO2'   | 22:DA:730:A:H8    | 1.66                     | 0.42              |
| 26:DE:155:GLU:O    | 26:DE:159:LEU:HG  | 2.20                     | 0.42              |
| 28:DG:95:ARG:HA    | 28:DG:128:GLN:O   | 2.19                     | 0.42              |
| 29:DH:121:VAL:O    | 29:DH:122:LEU:CB  | 2.67                     | 0.42              |
| 22:DA:1190:G:OP1   | 33:DL:32:GLY:HA2  | 2.20                     | 0.42              |
| 35:DN:116:VAL:HG13 | 35:DN:117:ASP:OD1 | 2.19                     | 0.42              |
| 35:DN:72:ASP:OD2   | 35:DN:75:ILE:HG12 | 2.20                     | 0.42              |
| 22:DA:85:G:OP2     | 42:DU:28:VAL:CG1  | 2.68                     | 0.42              |
| 42:DU:83:VAL:HG11  | 42:DU:94:ARG:HB3  | 2.02                     | 0.42              |
| 43:DV:48:MET:SD    | 43:DV:85:LYS:HA   | 2.59                     | 0.42              |
| 46:DY:2:LYS:O      | 46:DY:6:LEU:HB2   | 2.19                     | 0.42              |
| 1:AA:144:G:C4      | 1:AA:179:A:H2     | 2.36                     | 0.42              |
| 1:AA:167:A:H2'     | 1:AA:168:G:O4'    | 2.20                     | 0.42              |
| 1:AA:607:A:H2'     | 1:AA:608:A:C8     | 2.55                     | 0.42              |
| 1:AA:73:C:O2'      | 1:AA:74:A:P       | 2.78                     | 0.42              |
| 1:AA:787:A:C6      | 1:AA:788:U:C4     | 3.08                     | 0.42              |
| 1:AA:921:U:H2'     | 1:AA:922:G:O4'    | 2.20                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:AA:944:G:O2'     | 1:AA:1339:A:N6     | 2.53                     | 0.42              |
| 2:AB:131:LYS:HA    | 2:AB:131:LYS:HE2   | 2.02                     | 0.42              |
| 2:AB:80:VAL:HA     | 2:AB:214:LEU:HD21  | 2.01                     | 0.42              |
| 3:AC:22:TRP:HB3    | 3:AC:59:ARG:H      | 1.85                     | 0.42              |
| 4:AD:13:ARG:HD2    | 4:AD:34:ILE:HA     | 2.02                     | 0.42              |
| 4:AD:150:LYS:O     | 4:AD:151:LYS:C     | 2.57                     | 0.42              |
| 5:AE:105:ILE:HG13  | 5:AE:105:ILE:O     | 2.19                     | 0.42              |
| 5:AE:126:LYS:CD    | 5:AE:128:TYR:HE2   | 2.33                     | 0.42              |
| 6:AF:68:GLN:HA     | 6:AF:71:ILE:CG2    | 2.50                     | 0.42              |
| 6:AF:98:GLU:O      | 6:AF:99:ALA:O      | 2.38                     | 0.42              |
| 7:AG:27:VAL:HG23   | 7:AG:28:ASN:N      | 2.35                     | 0.42              |
| 8:AH:5:ASP:OD1     | 8:AH:8:ALA:HB2     | 2.20                     | 0.42              |
| 9:AI:57:MET:C      | 9:AI:59:GLU:N      | 2.73                     | 0.42              |
| 10:AJ:10:LEU:O     | 10:AJ:71:LEU:HA    | 2.19                     | 0.42              |
| 14:AN:7:LYS:O      | 14:AN:8:ALA:C      | 2.58                     | 0.42              |
| 10:AJ:63:ASP:OD1   | 14:AN:85:ARG:HD2   | 2.19                     | 0.42              |
| 14:AN:93:ILE:HG21  | 14:AN:96:LEU:HD22  | 2.02                     | 0.42              |
| 51:B3:8:ARG:O      | 51:B3:12:LYS:HG3   | 2.20                     | 0.42              |
| 53:B5:65:LEU:C     | 53:B5:65:LEU:HD13  | 2.40                     | 0.42              |
| 22:BA:1171:G:C2    | 22:BA:1179:G:N1    | 2.88                     | 0.42              |
| 22:BA:1442:U:H2'   | 22:BA:1443:U:C6    | 2.55                     | 0.42              |
| 22:BA:1483:G:C6    | 22:BA:1484:U:C4    | 3.08                     | 0.42              |
| 22:BA:17:G:H2'     | 22:BA:18:U:C6      | 2.54                     | 0.42              |
| 22:BA:1850:G:C2    | 22:BA:1893:C:O2    | 2.73                     | 0.42              |
| 22:BA:2672:U:C2'   | 22:BA:2673:G:O5'   | 2.68                     | 0.42              |
| 22:BA:2717:C:H2'   | 22:BA:2718:G:O4'   | 2.19                     | 0.42              |
| 22:BA:2839:G:C5    | 22:BA:2840:C:C5    | 3.07                     | 0.42              |
| 22:BA:2808:G:C2    | 22:BA:2891:U:C6    | 3.07                     | 0.42              |
| 55:BA:3001:DOL:O38 | 55:BA:3001:DOL:C29 | 2.68                     | 0.42              |
| 22:BA:54:G:H2'     | 22:BA:55:G:O5'     | 2.20                     | 0.42              |
| 26:BE:48:THR:HG23  | 26:BE:51:GLU:OE1   | 2.20                     | 0.42              |
| 22:BA:2311:A:C5    | 27:BF:77:PHE:HB3   | 2.55                     | 0.42              |
| 33:BL:23:ILE:O     | 33:BL:24:GLY:C     | 2.58                     | 0.42              |
| 36:BO:87:ILE:HG22  | 36:BO:88:LYS:N     | 2.34                     | 0.42              |
| 38:BQ:57:PHE:O     | 38:BQ:58:ARG:C     | 2.56                     | 0.42              |
| 40:BS:41:LYS:O     | 40:BS:44:ALA:N     | 2.52                     | 0.42              |
| 41:BT:57:VAL:CG2   | 41:BT:58:VAL:N     | 2.83                     | 0.42              |
| 43:BV:25:LYS:HE2   | 43:BV:43:ASP:CA    | 2.49                     | 0.42              |
| 45:BX:66:THR:O     | 45:BX:69:ALA:HB3   | 2.19                     | 0.42              |
| 46:BY:39:GLN:HB3   | 46:BY:41:HIS:CE1   | 2.54                     | 0.42              |
| 46:BY:61:ALA:O     | 46:BY:62:GLY:C     | 2.58                     | 0.42              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:CA:68:G:N2       | 1:CA:152:A:H1'     | 2.35                     | 0.42              |
| 1:CA:457:G:C5      | 1:CA:458:U:C4      | 3.08                     | 0.42              |
| 1:CA:801:U:N3      | 1:CA:802:A:N7      | 2.68                     | 0.42              |
| 1:CA:91:U:C4       | 1:CA:92:U:C4       | 3.08                     | 0.42              |
| 1:CA:990:C:C4      | 1:CA:991:U:O4      | 2.73                     | 0.42              |
| 2:CB:187:VAL:HG22  | 2:CB:187:VAL:O     | 2.20                     | 0.42              |
| 2:CB:207:ILE:HG12  | 2:CB:208:ARG:N     | 2.35                     | 0.42              |
| 2:CB:68:LEU:HD12   | 2:CB:158:PRO:CG    | 2.50                     | 0.42              |
| 2:CB:73:LYS:O      | 2:CB:74:ARG:C      | 2.57                     | 0.42              |
| 3:CC:167:TRP:C     | 3:CC:167:TRP:HE3   | 2.23                     | 0.42              |
| 6:CF:45:ARG:HD2    | 6:CF:59:TYR:CD2    | 2.54                     | 0.42              |
| 1:CA:1240:U:O4     | 7:CG:30:LEU:HG     | 2.20                     | 0.42              |
| 9:CI:21:ILE:HG22   | 9:CI:21:ILE:O      | 2.20                     | 0.42              |
| 1:CA:1280:A:O4'    | 10:CJ:43:PRO:HG3   | 2.19                     | 0.42              |
| 1:CA:1359:C:OP2    | 14:CN:75:ARG:NH1   | 2.53                     | 0.42              |
| 19:CS:74:PHE:CD1   | 19:CS:74:PHE:N     | 2.87                     | 0.42              |
| 22:DA:1221:C:H2'   | 22:DA:1222:U:O4'   | 2.20                     | 0.42              |
| 22:DA:1435:G:H2'   | 22:DA:1436:G:H5'   | 2.02                     | 0.42              |
| 22:DA:1312:U:C2    | 22:DA:1603:A:N1    | 2.88                     | 0.42              |
| 22:DA:1926:U:H5''  | 22:DA:1927:A:OP2   | 2.19                     | 0.42              |
| 22:DA:2167:U:O2    | 22:DA:2170:A:OP2   | 2.38                     | 0.42              |
| 22:DA:2553:G:H2'   | 22:DA:2554:U:H4'   | 2.02                     | 0.42              |
| 22:DA:1051:G:H4'   | 22:DA:2752:C:O2'   | 2.19                     | 0.42              |
| 22:DA:2800:A:H3'   | 22:DA:2801:G:H5'   | 2.02                     | 0.42              |
| 22:DA:2839:G:N2    | 22:DA:2880:C:C2    | 2.87                     | 0.42              |
| 22:DA:2864:G:C2'   | 22:DA:2865:U:H5'   | 2.50                     | 0.42              |
| 22:DA:2885:G:O6    | 48:D0:29:SER:HB3   | 2.20                     | 0.42              |
| 22:DA:54:G:C4      | 22:DA:55:G:C8      | 3.08                     | 0.42              |
| 22:DA:570:G:C2'    | 22:DA:571:U:H5'    | 2.49                     | 0.42              |
| 22:DA:584:C:N4     | 22:DA:585:G:O6     | 2.52                     | 0.42              |
| 22:DA:782:A:H4'    | 22:DA:783:A:O5'    | 2.19                     | 0.42              |
| 22:DA:796:C:H2'    | 22:DA:797:G:C8     | 2.55                     | 0.42              |
| 26:DE:192:ALA:O    | 26:DE:196:VAL:HG23 | 2.20                     | 0.42              |
| 26:DE:47:LYS:O     | 26:DE:83:VAL:HG11  | 2.20                     | 0.42              |
| 28:DG:121:ILE:HD12 | 28:DG:141:ILE:CG2  | 2.50                     | 0.42              |
| 28:DG:133:LEU:HD13 | 28:DG:141:ILE:HB   | 2.02                     | 0.42              |
| 28:DG:91:GLY:O     | 28:DG:92:VAL:O     | 2.37                     | 0.42              |
| 30:DI:33:VAL:O     | 30:DI:33:VAL:HG12  | 2.19                     | 0.42              |
| 30:DI:86:ILE:HD11  | 30:DI:89:GLY:HA2   | 2.01                     | 0.42              |
| 32:DK:31:ARG:CB    | 32:DK:32:TYR:CE2   | 3.03                     | 0.42              |
| 37:DP:70:VAL:HG12  | 37:DP:71:GLU:N     | 2.35                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 37:DP:30:VAL:HG22 | 37:DP:81:VAL:HA    | 2.01                     | 0.42              |
| 40:DS:30:SER:HA   | 40:DS:33:LEU:HD12  | 2.01                     | 0.42              |
| 22:DA:495:G:O4'   | 40:DS:57:ASN:ND2   | 2.53                     | 0.42              |
| 43:DV:51:GLN:HB3  | 43:DV:56:PHE:CD2   | 2.55                     | 0.42              |
| 45:DX:52:SER:O    | 45:DX:55:GLY:N     | 2.53                     | 0.42              |
| 1:AA:1128:C:H4'   | 1:AA:1148:U:O2     | 2.20                     | 0.41              |
| 1:AA:1130:A:C4    | 1:AA:1146:A:C2     | 3.08                     | 0.41              |
| 1:AA:1237:C:C4    | 1:AA:1336:C:N3     | 2.87                     | 0.41              |
| 1:AA:11:G:O2'     | 1:AA:12:U:H5'      | 2.20                     | 0.41              |
| 1:AA:1348:U:C5    | 1:AA:1373:G:N2     | 2.88                     | 0.41              |
| 1:AA:501:C:H2'    | 1:AA:502:A:H8      | 1.84                     | 0.41              |
| 1:AA:588:G:C6     | 1:AA:589:U:N3      | 2.88                     | 0.41              |
| 1:AA:588:G:N1     | 1:AA:589:U:C2      | 2.88                     | 0.41              |
| 1:AA:606:G:N3     | 1:AA:633:G:C6      | 2.88                     | 0.41              |
| 1:AA:945:G:C6     | 1:AA:1337:G:C5     | 3.08                     | 0.41              |
| 2:AB:118:GLU:O    | 2:AB:121:SER:CB    | 2.68                     | 0.41              |
| 2:AB:151:ILE:CD1  | 2:AB:154:MET:SD    | 3.06                     | 0.41              |
| 3:AC:6:HIS:CD2    | 3:AC:7:PRO:HD2     | 2.56                     | 0.41              |
| 4:AD:58:LYS:CE    | 4:AD:69:GLU:OE2    | 2.67                     | 0.41              |
| 5:AE:159:LYS:OXT  | 8:AH:64:LYS:NZ     | 2.51                     | 0.41              |
| 9:AI:44:ALA:O     | 9:AI:47:VAL:HG22   | 2.20                     | 0.41              |
| 9:AI:61:LEU:H     | 9:AI:61:LEU:HD23   | 1.85                     | 0.41              |
| 10:AJ:42:LEU:HA   | 10:AJ:43:PRO:HD2   | 1.83                     | 0.41              |
| 13:AM:111:GLY:O   | 13:AM:112:PRO:C    | 2.58                     | 0.41              |
| 13:AM:39:ILE:HG22 | 13:AM:40:ALA:N     | 2.34                     | 0.41              |
| 16:AP:45:GLU:O    | 16:AP:46:LYS:C     | 2.58                     | 0.41              |
| 19:AS:52:HIS:CD2  | 19:AS:54:GLY:N     | 2.88                     | 0.41              |
| 22:BA:1320:C:N3   | 22:BA:1331:G:O6    | 2.53                     | 0.41              |
| 22:BA:1357:C:H2'  | 22:BA:1357:C:O2    | 2.20                     | 0.41              |
| 22:BA:137:U:H2'   | 22:BA:140:C:N1     | 2.35                     | 0.41              |
| 22:BA:1491:G:N2   | 22:BA:1500:G:H1'   | 2.35                     | 0.41              |
| 22:BA:1922:G:C2   | 22:BA:1923:U:C6    | 3.07                     | 0.41              |
| 22:BA:2070:A:H2'  | 22:BA:2071:A:O4'   | 2.20                     | 0.41              |
| 22:BA:2402:U:C2'  | 22:BA:2403:C:OP2   | 2.68                     | 0.41              |
| 22:BA:2526:G:N3   | 52:B4:1:MET:N      | 2.68                     | 0.41              |
| 22:BA:2584:U:O2'  | 55:BA:3001:DOL:C48 | 2.66                     | 0.41              |
| 22:BA:2043:C:N3   | 22:BA:2777:G:C2    | 2.88                     | 0.41              |
| 22:BA:303:G:C5    | 22:BA:304:U:C5     | 3.07                     | 0.41              |
| 22:BA:545:U:C3'   | 22:BA:546:U:H4'    | 2.49                     | 0.41              |
| 22:BA:804:A:H5''  | 22:BA:805:G:OP1    | 2.20                     | 0.41              |
| 22:BA:825:A:H2'   | 22:BA:826:U:O4'    | 2.20                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:BA:918:A:H4'    | 23:BB:97:C:O2      | 2.19                     | 0.41              |
| 22:BA:971:G:H2'    | 22:BA:972:A:O4'    | 2.20                     | 0.41              |
| 22:BA:983:A:C6     | 22:BA:984:A:N1     | 2.88                     | 0.41              |
| 23:BB:33:G:C2'     | 23:BB:34:A:H5'     | 2.50                     | 0.41              |
| 24:BC:209:GLY:O    | 24:BC:212:ARG:HB2  | 2.20                     | 0.41              |
| 24:BC:237:GLY:CA   | 57:BC:407:HOH:O    | 2.66                     | 0.41              |
| 25:BD:157:LYS:HB2  | 25:BD:157:LYS:HE3  | 1.86                     | 0.41              |
| 25:BD:37:VAL:HG12  | 25:BD:38:LYS:N     | 2.35                     | 0.41              |
| 26:BE:112:LEU:HD13 | 26:BE:186:VAL:HG21 | 2.02                     | 0.41              |
| 28:BG:10:VAL:HG23  | 28:BG:48:ASN:O     | 2.20                     | 0.41              |
| 28:BG:48:ASN:C     | 28:BG:49:THR:HG23  | 2.40                     | 0.41              |
| 29:BH:104:THR:CG2  | 29:BH:110:VAL:O    | 2.68                     | 0.41              |
| 22:BA:1243:C:H1'   | 33:BL:4:ASN:O      | 2.20                     | 0.41              |
| 35:BN:55:ALA:HB2   | 35:BN:79:LEU:HB3   | 2.01                     | 0.41              |
| 22:BA:1266:G:N7    | 40:BS:16:LYS:HE3   | 2.35                     | 0.41              |
| 1:CA:1022:A:C5     | 1:CA:1023:U:C5     | 3.08                     | 0.41              |
| 1:CA:1144:G:C2     | 1:CA:1145:A:C2     | 3.07                     | 0.41              |
| 1:CA:1225:A:C2'    | 1:CA:1225:A:N3     | 2.83                     | 0.41              |
| 1:CA:1298:U:H4'    | 1:CA:1299:A:C4     | 2.54                     | 0.41              |
| 1:CA:978:A:O5'     | 1:CA:1362:A:N6     | 2.51                     | 0.41              |
| 1:CA:247:G:C6      | 1:CA:278:G:C2      | 3.08                     | 0.41              |
| 1:CA:451:A:OP2     | 16:CP:70:ARG:NH2   | 2.48                     | 0.41              |
| 1:CA:459:A:C2      | 1:CA:460:A:C5      | 3.08                     | 0.41              |
| 1:CA:570:G:C4      | 1:CA:571:U:C5      | 3.08                     | 0.41              |
| 1:CA:919:A:C2      | 1:CA:920:U:C6      | 3.08                     | 0.41              |
| 2:CB:55:ALA:O      | 2:CB:59:LYS:HB2    | 2.20                     | 0.41              |
| 6:CF:25:TYR:CD2    | 6:CF:25:TYR:N      | 2.84                     | 0.41              |
| 9:CI:26:GLY:CA     | 9:CI:61:LEU:O      | 2.68                     | 0.41              |
| 10:CJ:81:GLU:HA    | 10:CJ:84:VAL:HG12  | 2.02                     | 0.41              |
| 13:CM:46:SER:O     | 13:CM:47:GLU:HB3   | 2.19                     | 0.41              |
| 14:CN:58:SER:O     | 14:CN:59:ARG:HG3   | 2.20                     | 0.41              |
| 15:CO:89:ARG:CZ    | 22:DA:714:U:C5     | 3.03                     | 0.41              |
| 16:CP:71:VAL:O     | 16:CP:75:ILE:HD12  | 2.21                     | 0.41              |
| 17:CQ:15:ASP:O     | 17:CQ:17:MET:N     | 2.51                     | 0.41              |
| 20:CT:54:MET:CE    | 20:CT:58:VAL:HG21  | 2.50                     | 0.41              |
| 22:DA:1043:C:C5    | 22:DA:1044:C:C5    | 3.08                     | 0.41              |
| 22:DA:1222:U:H2'   | 22:DA:1223:G:C8    | 2.55                     | 0.41              |
| 22:DA:1305:C:N4    | 22:DA:1607:C:OP2   | 2.53                     | 0.41              |
| 22:DA:1764:C:C2'   | 22:DA:1765:U:H5'   | 2.50                     | 0.41              |
| 22:DA:1824:G:OP1   | 24:DC:53:HIS:CE1   | 2.73                     | 0.41              |
| 22:DA:1905:C:N4    | 22:DA:1930:G:C2    | 2.87                     | 0.41              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 22:DA:2061:G:C8    | 22:DA:2501:C:H4'  | 2.55                     | 0.41              |
| 22:DA:2322:A:C6    | 22:DA:2323:G:C5   | 3.08                     | 0.41              |
| 22:DA:2829:A:C2'   | 22:DA:2830:C:H5'  | 2.50                     | 0.41              |
| 22:DA:2847:U:C2'   | 22:DA:2848:G:H5'  | 2.50                     | 0.41              |
| 22:DA:2876:G:C6    | 22:DA:2877:G:C5   | 3.08                     | 0.41              |
| 22:DA:322:A:H3'    | 22:DA:323:C:C5'   | 2.50                     | 0.41              |
| 22:DA:294:A:N6     | 22:DA:345:A:N9    | 2.67                     | 0.41              |
| 22:DA:347:A:N6     | 22:DA:348:A:N6    | 2.68                     | 0.41              |
| 22:DA:287:G:N2     | 22:DA:354:A:C2    | 2.88                     | 0.41              |
| 22:DA:464:U:H2'    | 22:DA:465:G:O4'   | 2.20                     | 0.41              |
| 22:DA:470:A:C2     | 22:DA:471:A:C4    | 3.08                     | 0.41              |
| 22:DA:641:U:C5     | 22:DA:642:U:O4    | 2.73                     | 0.41              |
| 22:DA:669:G:N3     | 22:DA:801:G:C2    | 2.88                     | 0.41              |
| 22:DA:711:G:C2     | 22:DA:721:A:C2    | 3.08                     | 0.41              |
| 23:DB:46:A:C5      | 23:DB:47:C:C5     | 3.07                     | 0.41              |
| 24:DC:266:PHE:CD1  | 24:DC:266:PHE:N   | 2.87                     | 0.41              |
| 26:DE:56:GLY:O     | 26:DE:57:LYS:C    | 2.58                     | 0.41              |
| 28:DG:71:LEU:O     | 28:DG:75:MET:HG3  | 2.19                     | 0.41              |
| 29:DH:31:VAL:HB    | 29:DH:32:PRO:HD2  | 2.00                     | 0.41              |
| 30:DI:20:PRO:CG    | 30:DI:23:PRO:HG2  | 2.50                     | 0.41              |
| 32:DK:92:GLU:O     | 32:DK:93:GLN:HB2  | 2.19                     | 0.41              |
| 33:DL:127:VAL:HG12 | 33:DL:131:ALA:C   | 2.41                     | 0.41              |
| 22:DA:2334:U:O2'   | 36:DO:13:ARG:NH1  | 2.53                     | 0.41              |
| 38:DQ:58:ARG:CZ    | 38:DQ:92:ARG:NH1  | 2.83                     | 0.41              |
| 40:DS:10:ALA:HB3   | 40:DS:101:SER:O   | 2.20                     | 0.41              |
| 42:DU:99:ASN:ND2   | 42:DU:101:GLU:HB2 | 2.35                     | 0.41              |
| 42:DU:37:GLU:O     | 42:DU:37:GLU:HG3  | 2.19                     | 0.41              |
| 42:DU:59:VAL:HG12  | 42:DU:61:LYS:HD3  | 2.02                     | 0.41              |
| 1:AA:1044:A:C5     | 1:AA:1045:C:H1'   | 2.54                     | 0.41              |
| 1:AA:1121:U:H2'    | 1:AA:1122:U:O4'   | 2.20                     | 0.41              |
| 1:AA:1134:G:N2     | 1:AA:1135:U:O2    | 2.53                     | 0.41              |
| 1:AA:1286:U:O2     | 1:AA:1286:U:H2'   | 2.20                     | 0.41              |
| 1:AA:180:U:H2'     | 1:AA:181:A:O5'    | 2.19                     | 0.41              |
| 1:AA:203:G:O2'     | 1:AA:466:A:N1     | 2.53                     | 0.41              |
| 1:AA:666:G:C6      | 1:AA:741:G:C6     | 3.08                     | 0.41              |
| 1:AA:874:G:O2'     | 1:AA:875:U:H5'    | 2.20                     | 0.41              |
| 5:AE:41:ASP:OD1    | 5:AE:44:GLY:O     | 2.38                     | 0.41              |
| 5:AE:88:VAL:HG23   | 5:AE:93:ARG:HG2   | 2.02                     | 0.41              |
| 7:AG:87:VAL:HA     | 7:AG:88:PRO:HD3   | 1.92                     | 0.41              |
| 9:AI:5:GLN:OE1     | 9:AI:5:GLN:HA     | 2.20                     | 0.41              |
| 10:AJ:56:HIS:C     | 10:AJ:57:VAL:HG12 | 2.41                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 10:AJ:56:HIS:O    | 10:AJ:57:VAL:O     | 2.38                     | 0.41              |
| 13:AM:33:ILE:HG23 | 13:AM:59:GLU:HB3   | 2.02                     | 0.41              |
| 16:AP:45:GLU:O    | 16:AP:46:LYS:O     | 2.38                     | 0.41              |
| 16:AP:6:LEU:HD13  | 16:AP:71:VAL:HG23  | 2.01                     | 0.41              |
| 17:AQ:50:ASN:O    | 17:AQ:51:ASN:O     | 2.38                     | 0.41              |
| 17:AQ:61:ILE:CG2  | 17:AQ:73:TRP:CE3   | 3.03                     | 0.41              |
| 22:BA:2020:A:H5'  | 48:B0:9:THR:CG2    | 2.50                     | 0.41              |
| 22:BA:591:U:H1'   | 51:B3:2:PRO:N      | 2.35                     | 0.41              |
| 51:B3:55:LEU:O    | 51:B3:59:ILE:HG13  | 2.20                     | 0.41              |
| 22:BA:1196:C:O4'  | 22:BA:1226:A:C2    | 2.74                     | 0.41              |
| 22:BA:1269:A:O5'  | 22:BA:1269:A:H8    | 2.03                     | 0.41              |
| 22:BA:1588:G:C5   | 22:BA:1589:U:C5    | 3.08                     | 0.41              |
| 22:BA:163:C:H2'   | 22:BA:164:C:C6     | 2.54                     | 0.41              |
| 22:BA:1806:C:C2'  | 22:BA:1807:G:O5'   | 2.67                     | 0.41              |
| 22:BA:1887:C:H2'  | 22:BA:1888:G:O5'   | 2.20                     | 0.41              |
| 22:BA:1916:A:P    | 22:BA:1917:U:P     | 3.18                     | 0.41              |
| 22:BA:1990:C:H2'  | 22:BA:1991:U:C1'   | 2.50                     | 0.41              |
| 22:BA:2078:C:H2'  | 22:BA:2079:U:O4'   | 2.20                     | 0.41              |
| 22:BA:2345:G:C5   | 22:BA:2381:A:C2    | 3.08                     | 0.41              |
| 22:BA:2648:G:H2'  | 22:BA:2649:C:C6    | 2.55                     | 0.41              |
| 22:BA:2748:A:C2   | 22:BA:2757:A:C5    | 3.08                     | 0.41              |
| 22:BA:31:C:O2'    | 22:BA:1238:G:H5'   | 2.21                     | 0.41              |
| 22:BA:660:C:H2'   | 22:BA:661:A:H8     | 1.85                     | 0.41              |
| 22:BA:71:A:H5'    | 22:BA:73:A:C8      | 2.55                     | 0.41              |
| 22:BA:953:G:H5''  | 34:BM:16:ARG:NH1   | 2.35                     | 0.41              |
| 24:BC:142:HIS:HB2 | 24:BC:195:VAL:HG23 | 2.02                     | 0.41              |
| 22:BA:1819:A:OP1  | 24:BC:155:ALA:HA   | 2.20                     | 0.41              |
| 25:BD:26:VAL:HG22 | 25:BD:188:LEU:CD2  | 2.50                     | 0.41              |
| 25:BD:1:MET:HA    | 25:BD:88:GLU:OE1   | 2.20                     | 0.41              |
| 26:BE:7:ASP:C     | 26:BE:9:GLN:N      | 2.73                     | 0.41              |
| 29:BH:139:PHE:O   | 29:BH:140:ALA:HB3  | 2.20                     | 0.41              |
| 36:BO:92:PHE:HB2  | 36:BO:117:PHE:CD1  | 2.55                     | 0.41              |
| 1:CA:1261:A:C2    | 1:CA:1262:C:C5     | 3.08                     | 0.41              |
| 1:CA:1282:C:N3    | 1:CA:1283:U:C4     | 2.88                     | 0.41              |
| 1:CA:1282:C:H2'   | 1:CA:1282:C:O2     | 2.19                     | 0.41              |
| 1:CA:1289:A:O2'   | 7:CG:35:LYS:HE2    | 2.20                     | 0.41              |
| 1:CA:1408:A:C2    | 1:CA:1494:G:C2     | 3.08                     | 0.41              |
| 1:CA:1516:G:C2    | 1:CA:1518:A:OP2    | 2.73                     | 0.41              |
| 1:CA:313:A:H2'    | 1:CA:314:C:C6      | 2.55                     | 0.41              |
| 1:CA:50:A:H1'     | 1:CA:52:C:O4'      | 2.20                     | 0.41              |
| 2:CB:18:HIS:O     | 2:CB:19:GLN:HB2    | 2.19                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 2:CB:57:LEU:O     | 2:CB:60:ILE:CD1   | 2.68                     | 0.41              |
| 3:CC:81:GLY:O     | 3:CC:82:GLU:C     | 2.59                     | 0.41              |
| 4:CD:53:VAL:O     | 4:CD:54:GLN:C     | 2.58                     | 0.41              |
| 5:CE:104:GLY:HA3  | 5:CE:122:ASN:HA   | 2.01                     | 0.41              |
| 6:CF:38:ARG:HG3   | 6:CF:63:ASN:HB2   | 2.00                     | 0.41              |
| 7:CG:22:LEU:HG    | 7:CG:25:LYS:HE2   | 2.02                     | 0.41              |
| 9:CI:15:SER:OG    | 9:CI:70:GLY:HA3   | 2.19                     | 0.41              |
| 12:CL:90:LEU:HB2  | 12:CL:93:VAL:CG2  | 2.49                     | 0.41              |
| 16:CP:78:VAL:HG22 | 16:CP:78:VAL:O    | 2.20                     | 0.41              |
| 18:CR:72:ASP:C    | 18:CR:73:ARG:HG2  | 2.41                     | 0.41              |
| 11:CK:89:PRO:HD3  | 21:CU:29:LEU:CD1  | 2.51                     | 0.41              |
| 48:D0:10:ARG:HG2  | 48:D0:11:SER:N    | 2.35                     | 0.41              |
| 22:DA:1091:G:N2   | 22:DA:1092:C:C4   | 2.88                     | 0.41              |
| 22:DA:1193:G:C2   | 22:DA:1194:A:C5   | 3.08                     | 0.41              |
| 22:DA:1288:G:C8   | 22:DA:1327:A:C6   | 3.08                     | 0.41              |
| 22:DA:1331:G:O2'  | 22:DA:1332:G:H5'  | 2.20                     | 0.41              |
| 22:DA:1555:G:C2   | 22:DA:1556:C:C2   | 3.08                     | 0.41              |
| 22:DA:1343:G:C4   | 22:DA:1597:A:C6   | 3.09                     | 0.41              |
| 22:DA:1999:C:O2   | 22:DA:2687:U:O2'  | 2.33                     | 0.41              |
| 22:DA:2144:G:C2   | 22:DA:2146:C:O2   | 2.73                     | 0.41              |
| 22:DA:2238:G:C4'  | 22:DA:2239:G:OP1  | 2.68                     | 0.41              |
| 22:DA:2286:G:C4'  | 22:DA:2287:A:O5'  | 2.63                     | 0.41              |
| 22:DA:227:A:H4'   | 22:DA:228:C:OP1   | 2.20                     | 0.41              |
| 22:DA:2336:A:N3   | 22:DA:2385:C:H1'  | 2.35                     | 0.41              |
| 22:DA:2477:U:O4   | 52:D4:10:LEU:CD2  | 2.68                     | 0.41              |
| 22:DA:2718:G:C2   | 22:DA:2719:G:C1'  | 3.03                     | 0.41              |
| 22:DA:2784:U:H2'  | 22:DA:2785:C:C6   | 2.55                     | 0.41              |
| 22:DA:381:G:C2'   | 22:DA:382:A:H5'   | 2.50                     | 0.41              |
| 22:DA:265:A:N1    | 22:DA:427:U:O2'   | 2.53                     | 0.41              |
| 22:DA:82:U:N3     | 22:DA:83:A:N7     | 2.68                     | 0.41              |
| 22:DA:876:C:N4    | 22:DA:877:A:N6    | 2.68                     | 0.41              |
| 22:DA:875:G:N2    | 22:DA:903:C:C2    | 2.88                     | 0.41              |
| 25:DD:104:VAL:O   | 25:DD:105:LYS:HB3 | 2.20                     | 0.41              |
| 26:DE:100:MET:O   | 26:DE:104:ALA:CB  | 2.68                     | 0.41              |
| 27:DF:73:SER:HB2  | 27:DF:81:GLN:HB2  | 2.03                     | 0.41              |
| 29:DH:40:THR:OG1  | 29:DH:43:ASN:ND2  | 2.54                     | 0.41              |
| 36:DO:115:LEU:O   | 36:DO:117:PHE:N   | 2.48                     | 0.41              |
| 39:DR:87:GLN:HG2  | 39:DR:88:GLY:N    | 2.35                     | 0.41              |
| 1:AA:132:C:H2'    | 1:AA:133:U:O4'    | 2.21                     | 0.41              |
| 1:AA:748:G:N1     | 1:AA:749:A:C5     | 2.88                     | 0.41              |
| 1:AA:956:U:H2'    | 1:AA:957:U:O4'    | 2.20                     | 0.41              |

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| Atom-1            | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 2:AB:145:GLU:O    | 2:AB:149:GLY:N      | 2.54                     | 0.41              |
| 3:AC:3:GLN:OE1    | 3:AC:3:GLN:N        | 2.53                     | 0.41              |
| 3:AC:51:SER:O     | 3:AC:115:LEU:HD21   | 2.20                     | 0.41              |
| 6:AF:3:HIS:CA     | 6:AF:92:THR:HG23    | 2.50                     | 0.41              |
| 9:AI:80:ARG:NH1   | 9:AI:103:PHE:CE1    | 2.88                     | 0.41              |
| 10:AJ:56:HIS:O    | 10:AJ:57:VAL:CG1    | 2.68                     | 0.41              |
| 12:AL:32:GLY:HA3  | 12:AL:55:VAL:HG12   | 2.02                     | 0.41              |
| 16:AP:19:VAL:HG13 | 16:AP:38:PHE:N      | 2.35                     | 0.41              |
| 20:AT:44:LYS:CE   | 20:AT:87:ALA:HA     | 2.50                     | 0.41              |
| 48:B0:11:SER:O    | 48:B0:15:MET:HG3    | 2.20                     | 0.41              |
| 22:BA:1180:U:H2'  | 22:BA:1181:U:O4'    | 2.19                     | 0.41              |
| 22:BA:1203:U:O4   | 22:BA:1204:A:C6     | 2.73                     | 0.41              |
| 22:BA:136:G:N2    | 22:BA:144:A:C6      | 2.88                     | 0.41              |
| 22:BA:1739:A:H2'  | 22:BA:1740:G:O4'    | 2.19                     | 0.41              |
| 22:BA:1846:G:H2'  | 22:BA:1847:A:C4     | 2.55                     | 0.41              |
| 22:BA:2452:C:N3   | 55:BA:3001:DOL:H131 | 2.34                     | 0.41              |
| 22:BA:2714:G:O2'  | 22:BA:2715:C:H5'    | 2.20                     | 0.41              |
| 22:BA:281:C:H2'   | 22:BA:282:A:C8      | 2.55                     | 0.41              |
| 22:BA:393:C:H2'   | 22:BA:394:C:C6      | 2.55                     | 0.41              |
| 22:BA:785:G:C5    | 22:BA:786:C:C5      | 3.09                     | 0.41              |
| 22:BA:870:U:N3    | 22:BA:871:U:C5      | 2.89                     | 0.41              |
| 24:BC:166:ALA:HB3 | 24:BC:173:THR:HB    | 2.02                     | 0.41              |
| 27:BF:44:ILE:HG21 | 27:BF:79:ILE:HG22   | 2.01                     | 0.41              |
| 27:BF:92:ARG:N    | 27:BF:96:MET:HB2    | 2.35                     | 0.41              |
| 28:BG:74:SER:HA   | 28:BG:77:ILE:HG12   | 2.02                     | 0.41              |
| 30:BI:59:ILE:HG22 | 30:BI:61:VAL:HG23   | 2.01                     | 0.41              |
| 34:BM:55:ARG:CZ   | 34:BM:55:ARG:CB     | 2.99                     | 0.41              |
| 41:BT:12:ARG:CB   | 41:BT:33:LYS:O      | 2.68                     | 0.41              |
| 22:BA:309:A:H4'   | 42:BU:16:GLY:HA2    | 2.01                     | 0.41              |
| 42:BU:34:VAL:HG23 | 42:BU:65:ILE:HG22   | 2.01                     | 0.41              |
| 1:CA:1095:U:N3    | 1:CA:1096:C:C4      | 2.88                     | 0.41              |
| 1:CA:1159:U:H5''  | 1:CA:1159:U:O2      | 2.19                     | 0.41              |
| 1:CA:1243:C:H2'   | 1:CA:1244:G:C8      | 2.56                     | 0.41              |
| 1:CA:1262:C:N4    | 1:CA:1263:C:C4      | 2.88                     | 0.41              |
| 1:CA:1300:G:N1    | 1:CA:1335:U:C6      | 2.88                     | 0.41              |
| 1:CA:1394:A:H2'   | 1:CA:1501:C:O2'     | 2.20                     | 0.41              |
| 1:CA:28:A:H2'     | 1:CA:29:U:O4'       | 2.20                     | 0.41              |
| 1:CA:436:C:H2'    | 1:CA:437:U:C6       | 2.55                     | 0.41              |
| 1:CA:743:A:C5     | 1:CA:744:C:C5       | 3.08                     | 0.41              |
| 1:CA:785:G:N3     | 1:CA:785:G:H2'      | 2.34                     | 0.41              |
| 1:CA:842:U:O2'    | 1:CA:846:G:C6       | 2.73                     | 0.41              |

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| Atom-1              | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|--------------------|--------------------------|-------------------|
| 1:CA:857:C:H2'      | 1:CA:858:G:O4'     | 2.20                     | 0.41              |
| 1:CA:926:G:C6       | 1:CA:1505:G:C6     | 3.08                     | 0.41              |
| 1:CA:75:G:N2        | 1:CA:96:U:H1'      | 2.34                     | 0.41              |
| 1:CA:977:A:O2'      | 1:CA:1223:C:N4     | 2.52                     | 0.41              |
| 1:CA:980:C:OP1      | 57:CA:1866:HOH:O   | 2.22                     | 0.41              |
| 6:AF:15:SER:HB2     | 4:CD:193:ALA:CB    | 2.50                     | 0.41              |
| 1:CA:401:C:OP2      | 4:CD:70:ARG:HD3    | 2.20                     | 0.41              |
| 5:CE:38:VAL:HG12    | 5:CE:39:VAL:N      | 2.36                     | 0.41              |
| 9:CI:51:PRO:HG2     | 9:CI:83:ILE:HD12   | 2.02                     | 0.41              |
| 15:CO:35:GLN:NE2    | 15:CO:39:LEU:CD2   | 2.83                     | 0.41              |
| 1:CA:1458:G:O3'     | 20:CT:23:SER:HA    | 2.20                     | 0.41              |
| 20:CT:30:THR:O      | 20:CT:34:LYS:HG2   | 2.20                     | 0.41              |
| 22:DA:109:C:H5'     | 22:DA:348:A:O4'    | 2.20                     | 0.41              |
| 22:DA:121:G:H1'     | 22:DA:131:A:N1     | 2.35                     | 0.41              |
| 22:DA:1319:C:C2     | 22:DA:1334:G:C2    | 3.08                     | 0.41              |
| 22:DA:1537:G:N3     | 22:DA:1537:G:H3'   | 2.36                     | 0.41              |
| 22:DA:1623:G:C2     | 22:DA:1624:U:C6    | 3.08                     | 0.41              |
| 22:DA:1760:C:H2'    | 22:DA:1761:C:O4'   | 2.20                     | 0.41              |
| 22:DA:1847:A:O2'    | 22:DA:1848:A:P     | 2.77                     | 0.41              |
| 22:DA:1933:G:H2'    | 22:DA:1934:C:O4'   | 2.21                     | 0.41              |
| 22:DA:200:U:C5      | 22:DA:201:C:C5     | 3.09                     | 0.41              |
| 22:DA:2193:G:H2'    | 22:DA:2194:U:C6    | 2.55                     | 0.41              |
| 22:DA:2345:G:H5'    | 22:DA:2347:C:O4'   | 2.20                     | 0.41              |
| 22:DA:2896:C:H2'    | 22:DA:2897:U:O5'   | 2.20                     | 0.41              |
| 22:DA:290:U:N3      | 22:DA:291:G:C5     | 2.88                     | 0.41              |
| 55:DA:3001:DOL:H432 | 55:DA:3001:DOL:C1  | 2.49                     | 0.41              |
| 22:DA:372:G:H1'     | 22:DA:400:G:O6     | 2.20                     | 0.41              |
| 22:DA:435:C:H2'     | 22:DA:436:C:H5'    | 2.01                     | 0.41              |
| 22:DA:46:G:N3       | 22:DA:47:C:C6      | 2.88                     | 0.41              |
| 22:DA:485:C:H2'     | 22:DA:486:C:O4'    | 2.19                     | 0.41              |
| 22:DA:562:U:H2'     | 22:DA:572:A:O4'    | 2.20                     | 0.41              |
| 22:DA:581:C:H2'     | 22:DA:582:A:C8     | 2.55                     | 0.41              |
| 22:DA:878:A:C2      | 22:DA:900:A:C4     | 3.09                     | 0.41              |
| 23:DB:29:A:H2'      | 23:DB:30:C:O4'     | 2.20                     | 0.41              |
| 24:DC:17:VAL:HB     | 24:DC:204:VAL:HG22 | 2.02                     | 0.41              |
| 28:DG:80:THR:HG22   | 28:DG:81:GLU:N     | 2.35                     | 0.41              |
| 31:DJ:80:HIS:C      | 31:DJ:82:GLY:N     | 2.73                     | 0.41              |
| 33:DL:127:VAL:CG1   | 33:DL:131:ALA:C    | 2.89                     | 0.41              |
| 26:DE:29:HIS:CD2    | 33:DL:6:LEU:HB3    | 2.55                     | 0.41              |
| 33:DL:78:ARG:CB     | 33:DL:113:ALA:CB   | 2.98                     | 0.41              |
| 36:DO:92:PHE:HB2    | 36:DO:117:PHE:CD1  | 2.55                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 37:DP:49:ALA:HB3  | 37:DP:60:THR:OG1  | 2.21                     | 0.41              |
| 40:DS:18:ARG:HA   | 40:DS:21:ALA:HB3  | 2.02                     | 0.41              |
| 41:DT:38:ALA:C    | 41:DT:39:THR:HG22 | 2.41                     | 0.41              |
| 41:DT:34:VAL:HG11 | 41:DT:43:ILE:HD13 | 2.02                     | 0.41              |
| 1:AA:1074:G:C2    | 1:AA:1075:U:C2    | 3.08                     | 0.41              |
| 1:AA:1145:A:O2'   | 1:AA:1146:A:P     | 2.78                     | 0.41              |
| 1:AA:1238:A:H5'   | 1:AA:1336:C:H41   | 1.84                     | 0.41              |
| 1:AA:937:A:C2     | 1:AA:1379:G:O6    | 2.73                     | 0.41              |
| 1:AA:215:C:H2'    | 1:AA:216:U:O4'    | 2.21                     | 0.41              |
| 1:AA:338:A:H2'    | 1:AA:339:C:O4'    | 2.19                     | 0.41              |
| 1:AA:411:A:N7     | 1:AA:429:U:C5     | 2.89                     | 0.41              |
| 1:AA:454:G:C2'    | 1:AA:455:G:H5'    | 2.50                     | 0.41              |
| 1:AA:602:A:C2     | 1:AA:603:U:C2     | 3.09                     | 0.41              |
| 1:AA:676:A:C6     | 1:AA:677:U:C4     | 3.08                     | 0.41              |
| 1:AA:715:A:N6     | 1:AA:716:A:N6     | 2.69                     | 0.41              |
| 1:AA:872:A:N7     | 1:AA:874:G:C8     | 2.88                     | 0.41              |
| 2:AB:71:GLY:HA2   | 2:AB:164:ILE:CG2  | 2.51                     | 0.41              |
| 2:AB:47:VAL:C     | 2:AB:49:MET:N     | 2.74                     | 0.41              |
| 2:AB:96:TRP:O     | 2:AB:97:LEU:C     | 2.59                     | 0.41              |
| 4:AD:19:LEU:HD22  | 4:AD:64:ILE:HG13  | 2.02                     | 0.41              |
| 4:AD:61:VAL:O     | 4:AD:64:ILE:HB    | 2.20                     | 0.41              |
| 9:AI:85:ARG:O     | 9:AI:88:MET:HB2   | 2.20                     | 0.41              |
| 10:AJ:51:VAL:O    | 10:AJ:62:ARG:HA   | 2.20                     | 0.41              |
| 13:AM:109:ARG:O   | 13:AM:109:ARG:HG3 | 2.20                     | 0.41              |
| 13:AM:23:TYR:O    | 13:AM:69:LEU:HD23 | 2.20                     | 0.41              |
| 13:AM:58:ASP:O    | 13:AM:61:ALA:HB3  | 2.21                     | 0.41              |
| 13:AM:90:ARG:NH1  | 13:AM:95:LEU:HB3  | 2.35                     | 0.41              |
| 13:AM:2:ALA:C     | 13:AM:9:ILE:HG23  | 2.41                     | 0.41              |
| 17:AQ:15:ASP:HA   | 17:AQ:21:ILE:CD1  | 2.51                     | 0.41              |
| 21:AU:37:PHE:CD1  | 21:AU:40:LYS:HG2  | 2.55                     | 0.41              |
| 22:BA:1179:G:N7   | 22:BA:1180:U:N1   | 2.69                     | 0.41              |
| 22:BA:1206:G:C5   | 22:BA:1207:C:C4   | 3.09                     | 0.41              |
| 22:BA:1378:A:C4   | 22:BA:1380:G:C8   | 3.09                     | 0.41              |
| 22:BA:1456:G:C5   | 22:BA:1457:U:C5   | 3.08                     | 0.41              |
| 22:BA:195:A:C6    | 22:BA:198:C:C5    | 3.09                     | 0.41              |
| 22:BA:570:G:C4    | 22:BA:2030:A:N7   | 2.88                     | 0.41              |
| 22:BA:2191:A:C4   | 22:BA:2192:U:C4   | 3.09                     | 0.41              |
| 22:BA:2259:U:C6   | 22:BA:2427:C:C4   | 3.09                     | 0.41              |
| 22:BA:247:G:H4'   | 22:BA:386:G:C5    | 2.55                     | 0.41              |
| 22:BA:2502:G:C5'  | 22:BA:2503:A:C5'  | 2.99                     | 0.41              |
| 22:BA:2559:C:H2'  | 22:BA:2560:A:O5'  | 2.21                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:BA:257:C:H3'   | 22:BA:258:G:C8    | 2.55                     | 0.41              |
| 22:BA:2721:A:C2   | 22:BA:2873:A:C5   | 3.09                     | 0.41              |
| 22:BA:2765:A:C2'  | 22:BA:2765:A:N3   | 2.83                     | 0.41              |
| 22:BA:404:A:C8    | 22:BA:406:G:C6    | 3.07                     | 0.41              |
| 22:BA:494:G:C2'   | 22:BA:495:G:H5'   | 2.50                     | 0.41              |
| 22:BA:54:G:C2'    | 22:BA:55:G:O5'    | 2.68                     | 0.41              |
| 24:BC:165:VAL:O   | 24:BC:166:ALA:HB2 | 2.20                     | 0.41              |
| 26:BE:147:LEU:HB2 | 26:BE:183:PHE:CD1 | 2.55                     | 0.41              |
| 28:BG:55:ARG:HG2  | 28:BG:58:TYR:CD1  | 2.56                     | 0.41              |
| 29:BH:90:LEU:HD13 | 29:BH:125:THR:HA  | 2.03                     | 0.41              |
| 32:BK:53:LYS:HG3  | 32:BK:56:ASP:OD2  | 2.20                     | 0.41              |
| 37:BP:43:PHE:CE2  | 37:BP:63:LYS:HD3  | 2.56                     | 0.41              |
| 41:BT:18:GLU:O    | 41:BT:19:LYS:C    | 2.58                     | 0.41              |
| 42:BU:26:LYS:HA   | 42:BU:26:LYS:HD2  | 1.88                     | 0.41              |
| 43:BV:41:GLU:O    | 43:BV:41:GLU:HG2  | 2.18                     | 0.41              |
| 22:BA:78:U:OP2    | 46:BY:2:LYS:HD3   | 2.21                     | 0.41              |
| 22:BA:75:G:H4'    | 46:BY:48:ARG:NH2  | 2.34                     | 0.41              |
| 1:CA:312:C:H2'    | 1:CA:313:A:O4'    | 2.21                     | 0.41              |
| 1:CA:373:A:C2'    | 1:CA:374:A:H5'    | 2.50                     | 0.41              |
| 1:CA:496:A:H2'    | 1:CA:496:A:N3     | 2.35                     | 0.41              |
| 1:CA:545:C:O2'    | 1:CA:549:C:H5''   | 2.20                     | 0.41              |
| 1:CA:64:G:C2      | 1:CA:67:C:N4      | 2.88                     | 0.41              |
| 1:CA:64:G:N2      | 1:CA:67:C:C4      | 2.89                     | 0.41              |
| 1:CA:821:G:H2'    | 1:CA:822:U:C6     | 2.54                     | 0.41              |
| 1:CA:878:A:C5     | 1:CA:879:C:C5     | 3.08                     | 0.41              |
| 2:CB:60:ILE:HD12  | 2:CB:61:ALA:N     | 2.36                     | 0.41              |
| 3:CC:101:ILE:HG23 | 3:CC:101:ILE:O    | 2.20                     | 0.41              |
| 3:CC:153:VAL:HG23 | 3:CC:196:ILE:CG2  | 2.50                     | 0.41              |
| 4:CD:168:PRO:HB3  | 4:CD:171:LEU:HD12 | 2.00                     | 0.41              |
| 4:CD:188:ARG:O    | 4:CD:191:LEU:HD12 | 2.21                     | 0.41              |
| 5:CE:15:LEU:C     | 5:CE:16:ILE:HD12  | 2.41                     | 0.41              |
| 10:CJ:91:ASP:O    | 10:CJ:92:LEU:CB   | 2.68                     | 0.41              |
| 12:CL:90:LEU:HB2  | 12:CL:93:VAL:HG21 | 2.02                     | 0.41              |
| 13:CM:19:LEU:CD1  | 13:CM:33:ILE:HB   | 2.50                     | 0.41              |
| 17:CQ:48:ASP:O    | 17:CQ:49:GLU:C    | 2.57                     | 0.41              |
| 11:CK:112:ASP:HB3 | 21:CU:20:LYS:HE3  | 2.02                     | 0.41              |
| 49:D1:5:ILE:HG22  | 49:D1:28:ARG:CZ   | 2.50                     | 0.41              |
| 22:DA:1022:G:C6   | 22:DA:1140:C:C5   | 3.08                     | 0.41              |
| 22:DA:102:U:C2    | 46:DY:2:LYS:HE2   | 2.56                     | 0.41              |
| 22:DA:1360:G:O6   | 22:DA:1372:U:N3   | 2.53                     | 0.41              |
| 22:DA:1581:G:N7   | 22:DA:1582:C:N4   | 2.69                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:DA:167:A:H2'   | 22:DA:168:G:O4'    | 2.21                     | 0.41              |
| 22:DA:1710:G:O2'  | 22:DA:1711:A:H5'   | 2.21                     | 0.41              |
| 22:DA:781:A:H2'   | 22:DA:1777:U:O2'   | 2.19                     | 0.41              |
| 22:DA:17:G:C6     | 22:DA:524:G:C6     | 3.08                     | 0.41              |
| 22:DA:1866:A:C2   | 22:DA:1876:A:C5    | 3.07                     | 0.41              |
| 22:DA:191:A:C6    | 22:DA:192:C:N4     | 2.89                     | 0.41              |
| 22:DA:2010:G:H5'' | 40:DS:42:LYS:HB2   | 2.00                     | 0.41              |
| 22:DA:201:C:C4    | 22:DA:202:U:C5     | 3.08                     | 0.41              |
| 22:DA:2064:C:H4'  | 22:DA:2251:G:N2    | 2.35                     | 0.41              |
| 22:DA:2196:C:O2'  | 22:DA:2197:U:H5'   | 2.20                     | 0.41              |
| 22:DA:2271:G:H2'  | 22:DA:2272:U:C6    | 2.55                     | 0.41              |
| 22:DA:2391:G:OP2  | 51:D3:35:LYS:NZ    | 2.50                     | 0.41              |
| 22:DA:2428:G:H5'' | 22:DA:2429:G:P     | 2.60                     | 0.41              |
| 22:DA:2802:G:C6   | 22:DA:2803:G:C5    | 3.08                     | 0.41              |
| 22:DA:46:G:C2     | 22:DA:47:C:C4      | 3.09                     | 0.41              |
| 22:DA:609:A:C5    | 22:DA:610:C:C2     | 3.09                     | 0.41              |
| 22:DA:842:U:C4    | 22:DA:843:G:N7     | 2.88                     | 0.41              |
| 25:DD:32:ASN:N    | 25:DD:96:ILE:O     | 2.53                     | 0.41              |
| 26:DE:170:ARG:NH2 | 26:DE:176:ASP:OD1  | 2.52                     | 0.41              |
| 26:DE:45:ALA:HA   | 26:DE:87:ALA:O     | 2.21                     | 0.41              |
| 27:DF:135:GLN:HG2 | 27:DF:141:ILE:HG12 | 2.03                     | 0.41              |
| 22:DA:2314:A:O4'  | 27:DF:155:THR:HG21 | 2.19                     | 0.41              |
| 28:DG:109:PHE:CD2 | 28:DG:109:PHE:N    | 2.89                     | 0.41              |
| 28:DG:89:LEU:CD1  | 28:DG:162:VAL:HG22 | 2.51                     | 0.41              |
| 29:DH:135:HIS:CG  | 29:DH:136:SER:N    | 2.89                     | 0.41              |
| 31:DJ:84:ILE:O    | 31:DJ:85:LYS:C     | 2.59                     | 0.41              |
| 22:DA:2851:A:O2'  | 35:DN:64:ARG:NH2   | 2.51                     | 0.41              |
| 36:DO:48:LEU:C    | 36:DO:49:VAL:HG23  | 2.41                     | 0.41              |
| 44:DW:50:ASN:OD1  | 44:DW:63:ALA:CB    | 2.68                     | 0.41              |
| 1:AA:1000:A:N1    | 1:AA:1041:G:N1     | 2.69                     | 0.41              |
| 1:AA:1307:U:H2'   | 1:AA:1308:U:H6     | 1.85                     | 0.41              |
| 1:AA:1327:C:O2'   | 1:AA:1328:C:H5'    | 2.20                     | 0.41              |
| 1:AA:568:G:H2'    | 1:AA:569:C:H6      | 1.86                     | 0.41              |
| 1:AA:591:U:OP2    | 8:AH:31:LYS:CD     | 2.68                     | 0.41              |
| 1:AA:69:G:H5'     | 1:AA:70:U:P        | 2.61                     | 0.41              |
| 1:AA:935:A:C2     | 1:AA:936:C:N1      | 2.89                     | 0.41              |
| 2:AB:144:LEU:O    | 2:AB:148:LEU:HB2   | 2.20                     | 0.41              |
| 5:AE:56:VAL:O     | 5:AE:60:ILE:CG2    | 2.68                     | 0.41              |
| 8:AH:49:PHE:C     | 8:AH:49:PHE:CD1    | 2.93                     | 0.41              |
| 8:AH:89:LYS:HG3   | 8:AH:90:ASP:H      | 1.84                     | 0.41              |
| 1:AA:656:G:N2     | 15:AO:23:GLY:HA3   | 2.35                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 16:AP:12:LYS:O    | 16:AP:13:LYS:HB2   | 2.20                     | 0.41              |
| 19:AS:52:HIS:CD2  | 19:AS:54:GLY:H     | 2.39                     | 0.41              |
| 21:AU:14:VAL:CG1  | 21:AU:16:LEU:HD21  | 2.50                     | 0.41              |
| 49:B1:40:ASP:HB2  | 49:B1:49:TYR:OH    | 2.20                     | 0.41              |
| 22:BA:1070:A:N1   | 22:BA:1097:U:O2'   | 2.44                     | 0.41              |
| 22:BA:1406:U:N3   | 22:BA:1407:G:N7    | 2.68                     | 0.41              |
| 22:BA:1414:C:C5   | 22:BA:1415:U:C5    | 3.09                     | 0.41              |
| 22:BA:1494:A:H2'  | 22:BA:1495:A:C8    | 2.55                     | 0.41              |
| 22:BA:1592:C:C2'  | 22:BA:1593:A:H5'   | 2.50                     | 0.41              |
| 22:BA:2154:A:H2'  | 22:BA:2155:U:C6    | 2.55                     | 0.41              |
| 22:BA:2488:G:C2'  | 22:BA:2489:U:H5'   | 2.51                     | 0.41              |
| 22:BA:2496:C:C2'  | 22:BA:2497:A:O5'   | 2.69                     | 0.41              |
| 22:BA:257:C:H3'   | 22:BA:258:G:H8     | 1.85                     | 0.41              |
| 22:BA:2820:A:H2'  | 22:BA:2821:A:OP1   | 2.20                     | 0.41              |
| 22:BA:2861:U:O2   | 22:BA:2862:G:C8    | 2.74                     | 0.41              |
| 22:BA:368:A:C6    | 22:BA:369:U:C4     | 3.09                     | 0.41              |
| 22:BA:454:A:H4'   | 22:BA:455:C:OP2    | 2.20                     | 0.41              |
| 22:BA:48:G:N2     | 22:BA:49:A:N1      | 2.69                     | 0.41              |
| 22:BA:589:U:H2'   | 22:BA:590:A:H8     | 1.85                     | 0.41              |
| 22:BA:744:U:H2'   | 22:BA:745:G:O4'    | 2.20                     | 0.41              |
| 23:BB:113:C:H1'   | 36:BO:45:SER:O     | 2.20                     | 0.41              |
| 24:BC:111:LYS:O   | 24:BC:112:ALA:C    | 2.57                     | 0.41              |
| 24:BC:31:ALA:HA   | 24:BC:34:LEU:HD12  | 2.03                     | 0.41              |
| 26:BE:145:ASP:HA  | 26:BE:166:LYS:O    | 2.20                     | 0.41              |
| 27:BF:175:PHE:CE1 | 27:BF:177:PHE:CZ   | 3.08                     | 0.41              |
| 23:BB:54:G:N2     | 27:BF:26:MET:CE    | 2.83                     | 0.41              |
| 29:BH:33:GLN:O    | 29:BH:35:LYS:N     | 2.53                     | 0.41              |
| 30:BI:140:VAL:O   | 30:BI:140:VAL:HG13 | 2.20                     | 0.41              |
| 41:BT:29:THR:HG23 | 41:BT:86:THR:HG23  | 2.03                     | 0.41              |
| 42:BU:6:ARG:O     | 42:BU:9:ASP:HB2    | 2.20                     | 0.41              |
| 43:BV:14:LYS:CD   | 43:BV:18:ARG:HH11  | 2.33                     | 0.41              |
| 43:BV:6:ALA:HB2   | 43:BV:42:LEU:HD23  | 2.03                     | 0.41              |
| 44:BW:49:ALA:O    | 44:BW:50:ASN:HB2   | 2.21                     | 0.41              |
| 1:CA:1186:G:H4'   | 9:CI:112:GLU:CD    | 2.41                     | 0.41              |
| 1:CA:1332:A:H2'   | 1:CA:1333:A:O4'    | 2.21                     | 0.41              |
| 1:CA:66:A:C4'     | 1:CA:173:U:C4      | 3.03                     | 0.41              |
| 1:CA:406:G:C2     | 1:CA:407:U:C6      | 3.09                     | 0.41              |
| 1:CA:456:A:C6     | 1:CA:457:G:C5      | 3.09                     | 0.41              |
| 1:CA:858:G:N7     | 1:CA:869:G:N7      | 2.69                     | 0.41              |
| 2:CB:111:ILE:O    | 2:CB:114:LEU:HB3   | 2.21                     | 0.41              |
| 1:CA:429:U:O3'    | 4:CD:22:LYS:HE3    | 2.20                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:CD:57:GLU:OE1    | 4:CD:57:GLU:HA     | 2.20                     | 0.41              |
| 7:CG:92:ARG:HA     | 7:CG:92:ARG:HE     | 1.84                     | 0.41              |
| 14:CN:31:ILE:HG22  | 14:CN:32:SER:N     | 2.36                     | 0.41              |
| 17:CQ:13:VAL:CG1   | 17:CQ:22:VAL:HG13  | 2.50                     | 0.41              |
| 21:CU:4:ILE:HA     | 21:CU:20:LYS:HZ1   | 1.84                     | 0.41              |
| 22:DA:1124:G:O2'   | 52:D4:37:GLN:O     | 2.37                     | 0.41              |
| 22:DA:1006:C:H6    | 22:DA:1006:C:O5'   | 2.04                     | 0.41              |
| 22:DA:1184:U:OP1   | 47:DZ:30:ARG:HD2   | 2.19                     | 0.41              |
| 22:DA:116:C:C5'    | 22:DA:128:C:C5     | 3.03                     | 0.41              |
| 22:DA:1317:G:N2    | 22:DA:1336:A:N3    | 2.68                     | 0.41              |
| 22:DA:1341:G:C2    | 41:DT:84:TYR:CD2   | 3.08                     | 0.41              |
| 22:DA:1359:A:C2    | 22:DA:1360:G:H1'   | 2.56                     | 0.41              |
| 22:DA:1404:C:H2'   | 22:DA:1405:U:O5'   | 2.21                     | 0.41              |
| 22:DA:1854:A:O4'   | 22:DA:2233:U:H4'   | 2.20                     | 0.41              |
| 22:DA:2184:A:H2'   | 22:DA:2185:U:C6    | 2.55                     | 0.41              |
| 22:DA:2262:U:N3    | 22:DA:2279:G:C2    | 2.88                     | 0.41              |
| 22:DA:2331:G:C2    | 22:DA:2385:C:C2    | 3.08                     | 0.41              |
| 22:DA:2544:G:H2'   | 22:DA:2545:G:O4'   | 2.20                     | 0.41              |
| 22:DA:2718:G:OP1   | 37:DP:98:TYR:CD1   | 2.74                     | 0.41              |
| 22:DA:2785:C:H2'   | 22:DA:2786:U:O4'   | 2.20                     | 0.41              |
| 22:DA:2811:G:OP1   | 25:DD:62:LYS:N     | 2.53                     | 0.41              |
| 22:DA:28:A:H2'     | 22:DA:29:U:O4'     | 2.21                     | 0.41              |
| 22:DA:377:G:O6     | 22:DA:378:C:N4     | 2.54                     | 0.41              |
| 22:DA:764:A:N1     | 22:DA:1789:A:O2'   | 2.49                     | 0.41              |
| 24:DC:130:LEU:HD12 | 24:DC:135:ILE:HG13 | 2.03                     | 0.41              |
| 24:DC:75:PRO:O     | 24:DC:76:ALA:HB2   | 2.20                     | 0.41              |
| 25:DD:114:LYS:HE2  | 25:DD:196:ALA:HB1  | 2.03                     | 0.41              |
| 26:DE:12:LEU:HD23  | 26:DE:13:THR:N     | 2.35                     | 0.41              |
| 26:DE:188:MET:CE   | 26:DE:192:ALA:HB3  | 2.50                     | 0.41              |
| 26:DE:47:LYS:O     | 26:DE:83:VAL:CG1   | 2.69                     | 0.41              |
| 27:DF:57:LEU:HB2   | 27:DF:65:PRO:HG2   | 2.03                     | 0.41              |
| 28:DG:34:THR:HG22  | 28:DG:35:ARG:N     | 2.36                     | 0.41              |
| 30:DI:109:ILE:HG22 | 30:DI:109:ILE:O    | 2.20                     | 0.41              |
| 31:DJ:64:VAL:HG23  | 31:DJ:65:THR:N     | 2.36                     | 0.41              |
| 32:DK:97:THR:C     | 32:DK:98:ARG:HG2   | 2.41                     | 0.41              |
| 33:DL:77:ILE:HG22  | 33:DL:78:ARG:N     | 2.36                     | 0.41              |
| 33:DL:82:LEU:C     | 33:DL:82:LEU:HD23  | 2.41                     | 0.41              |
| 35:DN:12:ARG:CZ    | 35:DN:20:MET:HE3   | 2.50                     | 0.41              |
| 37:DP:103:ARG:HD3  | 37:DP:108:ALA:HB2  | 2.02                     | 0.41              |
| 37:DP:31:TRP:O     | 37:DP:32:VAL:HB    | 2.20                     | 0.41              |
| 40:DS:55:ILE:O     | 40:DS:58:ALA:HB3   | 2.21                     | 0.41              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 42:DU:82:ARG:O   | 42:DU:97:LYS:CG    | 2.69                     | 0.41              |
| 43:DV:75:GLN:HB2 | 43:DV:92:VAL:CG2   | 2.50                     | 0.41              |
| 1:AA:1147:C:H4'  | 9:AI:7:TYR:CE1     | 2.55                     | 0.41              |
| 1:AA:1048:G:N2   | 1:AA:1214:C:O2     | 2.54                     | 0.41              |
| 1:AA:1462:C:C2   | 1:AA:1463:U:C6     | 3.09                     | 0.41              |
| 1:AA:172:A:C6    | 1:AA:174:A:C8      | 3.09                     | 0.41              |
| 1:AA:21:G:H1'    | 1:AA:915:A:N6      | 2.36                     | 0.41              |
| 1:AA:65:A:C5     | 1:AA:381:C:C5      | 3.08                     | 0.41              |
| 1:AA:457:G:C6    | 1:AA:458:U:N3      | 2.88                     | 0.41              |
| 1:AA:595:A:C6    | 1:AA:641:U:C6      | 3.09                     | 0.41              |
| 1:AA:663:A:H5'   | 1:AA:836:G:OP1     | 2.20                     | 0.41              |
| 4:AD:197:GLU:CD  | 4:AD:197:GLU:H     | 2.24                     | 0.41              |
| 1:AA:426:U:H5''  | 4:AD:37:ALA:HB1    | 2.01                     | 0.41              |
| 8:AH:28:PRO:O    | 8:AH:33:LYS:NZ     | 2.48                     | 0.41              |
| 1:AA:1370:G:H5'' | 9:AI:111:VAL:HG21  | 2.03                     | 0.41              |
| 12:AL:24:LEU:CB  | 12:AL:59:ASN:HD22  | 2.33                     | 0.41              |
| 13:AM:6:GLY:HA3  | 13:AM:66:GLU:HG3   | 2.02                     | 0.41              |
| 17:AQ:45:HIS:CG  | 17:AQ:70:THR:HG22  | 2.56                     | 0.41              |
| 18:AR:23:TYR:CE1 | 18:AR:24:LYS:HG3   | 2.56                     | 0.41              |
| 22:BA:210:C:OP1  | 50:B2:29:GLN:NE2   | 2.53                     | 0.41              |
| 22:BA:250:G:OP2  | 51:B3:13:ARG:NH1   | 2.54                     | 0.41              |
| 22:BA:1575:C:H2' | 22:BA:1576:U:O4'   | 2.21                     | 0.41              |
| 22:BA:2414:G:O2' | 22:BA:2415:G:H5'   | 2.21                     | 0.41              |
| 22:BA:2043:C:C4  | 22:BA:2777:G:C2    | 3.09                     | 0.41              |
| 22:BA:388:G:N7   | 22:BA:390:U:C2'    | 2.84                     | 0.41              |
| 22:BA:833:A:OP2  | 33:BL:39:LYS:HE2   | 2.21                     | 0.41              |
| 24:BC:17:VAL:HB  | 24:BC:204:VAL:HG13 | 2.03                     | 0.41              |
| 24:BC:71:LYS:HB3 | 24:BC:96:TYR:HE2   | 1.84                     | 0.41              |
| 27:BF:13:VAL:O   | 27:BF:14:LYS:C     | 2.59                     | 0.41              |
| 34:BM:17:ASN:O   | 34:BM:38:ARG:HD3   | 2.21                     | 0.41              |
| 36:BO:102:ARG:O  | 36:BO:105:ALA:HB3  | 2.20                     | 0.41              |
| 38:BQ:66:ASN:CG  | 38:BQ:76:TYR:HB2   | 2.40                     | 0.41              |
| 42:BU:54:GLN:N   | 42:BU:55:PRO:HD2   | 2.35                     | 0.41              |
| 1:CA:1088:G:C4   | 1:CA:1089:G:C8     | 3.08                     | 0.41              |
| 1:CA:1089:G:C2   | 1:CA:1090:U:H1'    | 2.56                     | 0.41              |
| 1:CA:1106:G:N2   | 1:CA:1107:C:C2     | 2.89                     | 0.41              |
| 1:CA:1269:A:N7   | 1:CA:1270:G:H1'    | 2.35                     | 0.41              |
| 1:CA:1346:A:O3'  | 1:CA:1347:G:H4'    | 2.21                     | 0.41              |
| 1:CA:1431:A:C6   | 1:CA:1432:G:N1     | 2.89                     | 0.41              |
| 1:CA:144:G:C4    | 1:CA:179:A:C2      | 3.09                     | 0.41              |
| 1:CA:560:A:N7    | 1:CA:566:G:C4      | 2.89                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:CA:846:G:H2'    | 1:CA:846:G:N3     | 2.35                     | 0.41              |
| 4:CD:150:LYS:O    | 4:CD:152:GLN:OE1  | 2.39                     | 0.41              |
| 4:CD:50:ASP:O     | 4:CD:53:VAL:HG22  | 2.20                     | 0.41              |
| 5:CE:38:VAL:HG12  | 5:CE:117:VAL:CG2  | 2.50                     | 0.41              |
| 6:CF:55:HIS:O     | 6:CF:56:LYS:O     | 2.37                     | 0.41              |
| 9:CI:118:LEU:CD1  | 9:CI:118:LEU:N    | 2.84                     | 0.41              |
| 9:CI:35:LEU:HD21  | 9:CI:48:VAL:HG21  | 2.02                     | 0.41              |
| 19:CS:79:THR:O    | 19:CS:79:THR:OG1  | 2.33                     | 0.41              |
| 20:CT:33:LYS:HA   | 20:CT:36:TYR:HD2  | 1.86                     | 0.41              |
| 22:DA:2015:A:C6   | 48:D0:3:VAL:HG23  | 2.55                     | 0.41              |
| 48:D0:40:ARG:O    | 48:D0:41:HIS:HB2  | 2.21                     | 0.41              |
| 50:D2:11:LYS:O    | 50:D2:15:SER:N    | 2.53                     | 0.41              |
| 50:D2:34:ARG:HB2  | 50:D2:42:LEU:CD1  | 2.51                     | 0.41              |
| 22:DA:1073:A:H2'  | 22:DA:1074:G:H5'  | 2.03                     | 0.41              |
| 22:DA:56:A:C2     | 22:DA:115:C:C2    | 3.08                     | 0.41              |
| 22:DA:1362:C:N4   | 22:DA:1363:C:C4   | 2.89                     | 0.41              |
| 22:DA:1378:A:H4'  | 22:DA:1379:U:OP1  | 2.20                     | 0.41              |
| 22:DA:1605:C:C4'  | 22:DA:1610:A:C6   | 3.03                     | 0.41              |
| 22:DA:1663:G:H3'  | 57:DA:3423:HOH:O  | 2.21                     | 0.41              |
| 22:DA:171:U:H2'   | 22:DA:172:A:C8    | 2.55                     | 0.41              |
| 22:DA:1731:G:H2'  | 22:DA:1732:C:H3'  | 2.02                     | 0.41              |
| 22:DA:2140:G:C6   | 22:DA:2152:G:C5   | 3.08                     | 0.41              |
| 22:DA:2205:A:C2   | 22:DA:2206:C:C2   | 3.08                     | 0.41              |
| 22:DA:2280:G:O2'  | 22:DA:2388:A:N1   | 2.40                     | 0.41              |
| 22:DA:2413:G:O2'  | 22:DA:2414:G:H5'  | 2.20                     | 0.41              |
| 22:DA:792:A:O2'   | 22:DA:2440:C:N3   | 2.42                     | 0.41              |
| 22:DA:245:G:O6    | 51:D3:8:ARG:CD    | 2.68                     | 0.41              |
| 22:DA:447:A:C8    | 22:DA:473:G:C6    | 3.08                     | 0.41              |
| 22:DA:485:C:C4    | 22:DA:496:G:C6    | 3.08                     | 0.41              |
| 22:DA:536:G:H2'   | 22:DA:537:G:O4'   | 2.21                     | 0.41              |
| 22:DA:612:G:H2'   | 22:DA:614:A:C8    | 2.55                     | 0.41              |
| 22:DA:683:U:H2'   | 22:DA:684:G:O5'   | 2.20                     | 0.41              |
| 22:DA:752:A:N3    | 22:DA:752:A:H2'   | 2.36                     | 0.41              |
| 22:DA:770:G:O4'   | 22:DA:1379:U:C5   | 2.74                     | 0.41              |
| 22:DA:900:A:C6    | 22:DA:901:C:C2    | 3.09                     | 0.41              |
| 22:DA:920:A:C5    | 22:DA:921:C:C5    | 3.08                     | 0.41              |
| 22:DA:947:A:H2'   | 22:DA:948:C:C6    | 2.56                     | 0.41              |
| 25:DD:114:LYS:HG2 | 25:DD:196:ALA:HB2 | 2.02                     | 0.41              |
| 26:DE:40:ARG:CZ   | 26:DE:92:HIS:CE1  | 3.03                     | 0.41              |
| 27:DF:74:VAL:CG2  | 27:DF:79:ILE:HD11 | 2.51                     | 0.41              |
| 29:DH:130:VAL:CG1 | 29:DH:131:SER:N   | 2.82                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 29:DH:53:GLU:C    | 29:DH:55:GLU:N    | 2.72                     | 0.41              |
| 22:DA:2848:G:C8   | 37:DP:95:ALA:HB2  | 2.55                     | 0.41              |
| 44:DW:37:ILE:HG22 | 44:DW:38:VAL:CG2  | 2.51                     | 0.41              |
| 1:AA:1014:A:C4    | 19:AS:34:TRP:CZ3  | 3.08                     | 0.41              |
| 1:AA:1099:G:C5    | 1:AA:1100:C:C5    | 3.08                     | 0.41              |
| 1:AA:1140:C:HO2'  | 1:AA:1141:C:P     | 2.44                     | 0.41              |
| 1:AA:1162:C:H2'   | 1:AA:1163:A:O4'   | 2.21                     | 0.41              |
| 1:AA:1195:C:H2'   | 1:AA:1197:A:O4'   | 2.20                     | 0.41              |
| 1:AA:1299:A:C6    | 1:AA:1301:U:O2    | 2.74                     | 0.41              |
| 1:AA:18:C:H2'     | 1:AA:19:A:O4'     | 2.21                     | 0.41              |
| 1:AA:238:A:H2'    | 1:AA:239:U:O4'    | 2.21                     | 0.41              |
| 1:AA:855:U:C4     | 1:AA:856:C:C5     | 3.08                     | 0.41              |
| 2:AB:27:MET:HE3   | 2:AB:193:PRO:HG3  | 2.02                     | 0.41              |
| 2:AB:9:MET:SD     | 2:AB:9:MET:N      | 2.94                     | 0.41              |
| 3:AC:175:LEU:O    | 3:AC:175:LEU:HD12 | 2.21                     | 0.41              |
| 4:AD:143:VAL:O    | 4:AD:143:VAL:CG2  | 2.65                     | 0.41              |
| 4:AD:88:GLU:HG2   | 4:AD:188:ARG:HD3  | 2.01                     | 0.41              |
| 8:AH:26:THR:O     | 8:AH:27:MET:HB3   | 2.21                     | 0.41              |
| 8:AH:2:SER:N      | 8:AH:4:GLN:HG3    | 2.36                     | 0.41              |
| 1:AA:1308:U:OP2   | 13:AM:98:ARG:HG3  | 2.21                     | 0.41              |
| 16:AP:51:ARG:NH1  | 16:AP:51:ARG:HB3  | 2.35                     | 0.41              |
| 16:AP:78:VAL:HG13 | 16:AP:78:VAL:O    | 2.20                     | 0.41              |
| 17:AQ:43:LYS:O    | 17:AQ:44:LEU:HD23 | 2.21                     | 0.41              |
| 20:AT:51:PHE:CD1  | 20:AT:51:PHE:C    | 2.93                     | 0.41              |
| 21:AU:25:LYS:O    | 21:AU:27:GLY:N    | 2.53                     | 0.41              |
| 49:B1:35:GLU:HA   | 49:B1:49:TYR:O    | 2.21                     | 0.41              |
| 22:BA:1001:A:P    | 57:BA:3736:HOH:O  | 2.73                     | 0.41              |
| 22:BA:1350:C:N3   | 22:BA:1382:G:C2   | 2.88                     | 0.41              |
| 22:BA:1424:G:C2   | 22:BA:1425:G:H1'  | 2.56                     | 0.41              |
| 22:BA:1584:U:OP1  | 22:BA:1584:U:C6   | 2.73                     | 0.41              |
| 22:BA:1688:U:O2   | 22:BA:1688:U:H2'  | 2.20                     | 0.41              |
| 22:BA:1879:C:H2'  | 22:BA:1880:U:O4'  | 2.20                     | 0.41              |
| 22:BA:2166:U:O4   | 22:BA:2170:A:N7   | 2.54                     | 0.41              |
| 22:BA:2243:U:O2'  | 22:BA:2244:U:H5'  | 2.20                     | 0.41              |
| 22:BA:2271:G:H2'  | 22:BA:2272:U:H6   | 1.86                     | 0.41              |
| 22:BA:2534:A:C2'  | 22:BA:2535:G:O5'  | 2.69                     | 0.41              |
| 22:BA:2592:G:C5   | 22:BA:2593:U:C4   | 3.09                     | 0.41              |
| 22:BA:221:A:C4    | 22:BA:266:G:N7    | 2.88                     | 0.41              |
| 22:BA:439:A:H2'   | 22:BA:440:C:O4'   | 2.19                     | 0.41              |
| 22:BA:499:U:O4    | 22:BA:500:G:C6    | 2.73                     | 0.41              |
| 22:BA:779:U:H2'   | 22:BA:779:U:O2    | 2.21                     | 0.41              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 23:BB:46:A:H2'     | 23:BB:47:C:O4'     | 2.21                     | 0.41              |
| 24:BC:199:GLU:O    | 24:BC:200:HIS:C    | 2.58                     | 0.41              |
| 26:BE:134:LEU:HD23 | 26:BE:160:ALA:O    | 2.19                     | 0.41              |
| 22:BA:2444:G:OP2   | 26:BE:63:LYS:HD3   | 2.20                     | 0.41              |
| 27:BF:14:LYS:O     | 27:BF:18:THR:CG2   | 2.69                     | 0.41              |
| 29:BH:30:LEU:C     | 29:BH:32:PRO:HD2   | 2.41                     | 0.41              |
| 29:BH:82:SER:HB3   | 29:BH:146:VAL:HG12 | 2.03                     | 0.41              |
| 30:BI:127:ARG:HA   | 30:BI:130:GLU:HG3  | 2.02                     | 0.41              |
| 34:BM:58:LYS:C     | 34:BM:60:GLN:H     | 2.24                     | 0.41              |
| 37:BP:53:ARG:NH1   | 37:BP:53:ARG:CG    | 2.75                     | 0.41              |
| 40:BS:36:LEU:HD13  | 40:BS:48:LYS:HA    | 2.01                     | 0.41              |
| 41:BT:29:THR:HG23  | 41:BT:86:THR:N     | 2.35                     | 0.41              |
| 41:BT:47:VAL:CG1   | 41:BT:55:VAL:CG2   | 2.99                     | 0.41              |
| 43:BV:80:HIS:ND1   | 43:BV:83:LYS:CG    | 2.84                     | 0.41              |
| 45:BX:18:ARG:CZ    | 45:BX:24:ALA:HB2   | 2.51                     | 0.41              |
| 1:CA:1000:A:H3'    | 1:CA:1001:C:C6     | 2.56                     | 0.41              |
| 1:CA:164:G:H2'     | 1:CA:164:G:N3      | 2.35                     | 0.41              |
| 1:CA:257:G:C2      | 1:CA:270:A:C6      | 3.08                     | 0.41              |
| 1:CA:382:A:H2'     | 1:CA:383:A:C8      | 2.55                     | 0.41              |
| 1:CA:587:G:H4'     | 8:CH:4:GLN:HA      | 2.03                     | 0.41              |
| 1:CA:792:A:H1'     | 1:CA:794:A:N7      | 2.35                     | 0.41              |
| 1:CA:79:G:N2       | 1:CA:91:U:O2       | 2.54                     | 0.41              |
| 1:CA:972:C:H4'     | 10:CJ:59:LYS:CG    | 2.50                     | 0.41              |
| 2:CB:115:LYS:HA    | 2:CB:118:GLU:HG2   | 2.03                     | 0.41              |
| 2:CB:87:CYS:SG     | 2:CB:89:GLN:NE2    | 2.94                     | 0.41              |
| 4:CD:76:TYR:O      | 4:CD:77:LYS:C      | 2.58                     | 0.41              |
| 7:CG:133:THR:HA    | 7:CG:136:LYS:HB3   | 2.03                     | 0.41              |
| 10:CJ:78:GLU:HA    | 10:CJ:79:PRO:HD3   | 1.89                     | 0.41              |
| 11:CK:52:PHE:CE2   | 11:CK:62:ALA:HB1   | 2.55                     | 0.41              |
| 13:CM:22:ILE:HG22  | 13:CM:23:TYR:N     | 2.36                     | 0.41              |
| 13:CM:81:MET:O     | 13:CM:83:LEU:N     | 2.53                     | 0.41              |
| 15:CO:43:PHE:CZ    | 15:CO:53:ARG:HA    | 2.56                     | 0.41              |
| 18:CR:20:GLU:O     | 18:CR:21:ILE:C     | 2.57                     | 0.41              |
| 48:D0:27:SER:O     | 48:D0:28:LEU:C     | 2.59                     | 0.41              |
| 22:DA:1040:A:H2'   | 22:DA:1041:G:O4'   | 2.20                     | 0.41              |
| 22:DA:1120:G:C5    | 22:DA:1121:C:C5    | 3.09                     | 0.41              |
| 22:DA:1231:U:C2'   | 22:DA:1232:G:H8    | 2.33                     | 0.41              |
| 22:DA:1366:A:C4    | 22:DA:1367:A:C8    | 3.09                     | 0.41              |
| 22:DA:1866:A:N7    | 22:DA:1867:G:C8    | 2.88                     | 0.41              |
| 22:DA:2179:C:H2'   | 22:DA:2180:U:C6    | 2.55                     | 0.41              |
| 22:DA:218:A:H2'    | 22:DA:219:A:O4'    | 2.21                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:DA:2314:A:C2   | 22:DA:2315:G:C5    | 3.09                     | 0.41              |
| 22:DA:232:G:N1    | 22:DA:420:C:OP1    | 2.53                     | 0.41              |
| 22:DA:251:A:H4'   | 33:DL:47:ARG:NH2   | 2.35                     | 0.41              |
| 22:DA:772:C:H2'   | 22:DA:773:U:O4'    | 2.20                     | 0.41              |
| 22:DA:804:A:H2'   | 22:DA:806:C:C4     | 2.56                     | 0.41              |
| 23:DB:29:A:C2     | 23:DB:30:C:C2      | 3.09                     | 0.41              |
| 23:DB:55:U:H4'    | 27:DF:25:VAL:HG12  | 2.02                     | 0.41              |
| 24:DC:129:THR:CG2 | 24:DC:130:LEU:N    | 2.83                     | 0.41              |
| 25:DD:106:LYS:HB2 | 25:DD:206:ALA:HB2  | 2.02                     | 0.41              |
| 27:DF:111:ILE:HB  | 27:DF:114:PHE:CB   | 2.51                     | 0.41              |
| 28:DG:91:GLY:O    | 28:DG:92:VAL:C     | 2.58                     | 0.41              |
| 30:DI:29:GLY:HA2  | 30:DI:33:VAL:HB    | 2.03                     | 0.41              |
| 30:DI:57:VAL:HG22 | 30:DI:69:PHE:HB2   | 2.02                     | 0.41              |
| 22:DA:2250:G:C2   | 34:DM:82:MET:CB    | 3.03                     | 0.41              |
| 36:DO:48:LEU:O    | 36:DO:49:VAL:CG2   | 2.69                     | 0.41              |
| 40:DS:47:VAL:HB   | 40:DS:103:ILE:HG21 | 2.02                     | 0.41              |
| 40:DS:95:ARG:CG   | 40:DS:95:ARG:O     | 2.68                     | 0.41              |
| 41:DT:38:ALA:O    | 41:DT:39:THR:CB    | 2.67                     | 0.41              |
| 41:DT:8:LEU:CD2   | 41:DT:50:LEU:HD21  | 2.50                     | 0.41              |
| 41:DT:77:ARG:O    | 41:DT:78:SER:HB2   | 2.21                     | 0.41              |
| 42:DU:21:LYS:HB2  | 42:DU:39:ILE:HD12  | 2.02                     | 0.41              |
| 43:DV:42:LEU:N    | 43:DV:42:LEU:HD23  | 2.36                     | 0.41              |
| 43:DV:49:ASN:O    | 43:DV:52:ALA:HB3   | 2.21                     | 0.41              |
| 45:DX:39:TRP:HB2  | 45:DX:46:PHE:CE2   | 2.56                     | 0.41              |
| 46:DY:20:ASN:O    | 46:DY:24:GLU:HB2   | 2.20                     | 0.41              |
| 1:AA:1125:U:C5    | 1:AA:1127:G:C5     | 3.09                     | 0.41              |
| 1:AA:1314:C:N4    | 19:AS:4:SER:HA     | 2.35                     | 0.41              |
| 1:AA:409:U:H2'    | 1:AA:410:G:O4'     | 2.21                     | 0.41              |
| 1:AA:464:U:N3     | 1:AA:467:U:OP2     | 2.50                     | 0.41              |
| 1:AA:675:A:OP1    | 18:AR:71:THR:HG21  | 2.21                     | 0.41              |
| 1:AA:676:A:C2     | 1:AA:677:U:C2      | 3.09                     | 0.41              |
| 1:AA:721:G:C6     | 1:AA:733:G:C2      | 3.09                     | 0.41              |
| 2:AB:210:VAL:O    | 2:AB:211:THR:C     | 2.59                     | 0.41              |
| 2:AB:41:ILE:N     | 2:AB:41:ILE:CD1    | 2.83                     | 0.41              |
| 9:AI:86:ALA:O     | 9:AI:88:MET:N      | 2.54                     | 0.41              |
| 1:AA:691:G:O6     | 11:AK:57:LYS:HE2   | 2.20                     | 0.41              |
| 12:AL:38:TYR:O    | 12:AL:39:THR:CG2   | 2.69                     | 0.41              |
| 13:AM:64:VAL:CG1  | 13:AM:64:VAL:O     | 2.63                     | 0.41              |
| 14:AN:64:CYS:HB2  | 14:AN:80:SER:HB2   | 2.03                     | 0.41              |
| 16:AP:21:VAL:HG21 | 16:AP:60:TRP:CD1   | 2.56                     | 0.41              |
| 16:AP:38:PHE:CE2  | 16:AP:51:ARG:HB2   | 2.56                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 50:B2:30:VAL:O    | 50:B2:34:ARG:HG3  | 2.20                     | 0.41              |
| 22:BA:1071:G:O4'  | 22:BA:1089:A:N7   | 2.53                     | 0.41              |
| 22:BA:1140:C:O4'  | 22:BA:1143:A:C2   | 2.73                     | 0.41              |
| 22:BA:1735:A:C4   | 22:BA:1736:U:C6   | 3.08                     | 0.41              |
| 22:BA:2779:U:C5   | 22:BA:2781:A:C2   | 3.09                     | 0.41              |
| 22:BA:2816:G:O3'  | 35:BN:99:LYS:HE2  | 2.21                     | 0.41              |
| 22:BA:359:G:H2'   | 22:BA:360:U:O4'   | 2.21                     | 0.41              |
| 22:BA:629:G:N3    | 22:BA:639:U:O2'   | 2.51                     | 0.41              |
| 22:BA:826:U:H2'   | 22:BA:828:U:O4'   | 2.21                     | 0.41              |
| 22:BA:999:U:H5    | 22:BA:1154:G:N7   | 2.19                     | 0.41              |
| 23:BB:101:A:H2'   | 23:BB:102:G:O4'   | 2.21                     | 0.41              |
| 23:BB:30:C:C2'    | 23:BB:31:C:H5'    | 2.48                     | 0.41              |
| 24:BC:71:LYS:HE3  | 24:BC:96:TYR:CD2  | 2.56                     | 0.41              |
| 29:BH:100:ALA:HB2 | 29:BH:115:VAL:CG2 | 2.50                     | 0.41              |
| 29:BH:95:GLY:HA2  | 29:BH:117:LEU:CD2 | 2.51                     | 0.41              |
| 31:BJ:80:HIS:O    | 31:BJ:81:ILE:C    | 2.58                     | 0.41              |
| 32:BK:41:ILE:HD11 | 32:BK:58:LEU:CD2  | 2.51                     | 0.41              |
| 22:BA:2392:A:O2'  | 33:BL:60:ARG:O    | 2.36                     | 0.41              |
| 33:BL:87:GLY:O    | 33:BL:89:VAL:HG12 | 2.21                     | 0.41              |
| 34:BM:95:LEU:C    | 34:BM:96:ILE:HD13 | 2.40                     | 0.41              |
| 35:BN:46:ARG:O    | 35:BN:50:PRO:HG2  | 2.21                     | 0.41              |
| 39:BR:69:GLY:C    | 39:BR:70:GLU:O    | 2.58                     | 0.41              |
| 42:BU:77:THR:O    | 42:BU:79:LYS:HG2  | 2.20                     | 0.41              |
| 46:BY:57:LEU:O    | 46:BY:57:LEU:CG   | 2.69                     | 0.41              |
| 1:CA:101:A:C5     | 1:CA:102:G:N7     | 2.88                     | 0.41              |
| 1:CA:375:U:C4     | 1:CA:376:G:N7     | 2.89                     | 0.41              |
| 1:CA:40:C:H2'     | 1:CA:41:G:O4'     | 2.20                     | 0.41              |
| 1:CA:414:A:N1     | 1:CA:415:A:C4     | 2.89                     | 0.41              |
| 1:CA:834:U:H2'    | 1:CA:835:U:C6     | 2.56                     | 0.41              |
| 1:CA:913:A:H4'    | 1:CA:914:A:H4'    | 2.03                     | 0.41              |
| 3:CC:179:ARG:O    | 3:CC:206:GLU:O    | 2.38                     | 0.41              |
| 4:CD:149:ALA:O    | 4:CD:150:LYS:C    | 2.56                     | 0.41              |
| 4:CD:153:SER:O    | 4:CD:154:ARG:C    | 2.58                     | 0.41              |
| 5:CE:134:ILE:HD12 | 5:CE:134:ILE:H    | 1.85                     | 0.41              |
| 5:CE:153:VAL:HG23 | 5:CE:153:VAL:O    | 2.20                     | 0.41              |
| 5:CE:36:LEU:HD21  | 5:CE:137:VAL:CG1  | 2.50                     | 0.41              |
| 8:CH:78:VAL:N     | 8:CH:126:ILE:O    | 2.51                     | 0.41              |
| 9:CI:13:LYS:O     | 9:CI:14:SER:CB    | 2.69                     | 0.41              |
| 11:CK:100:LEU:O   | 11:CK:101:ASN:C   | 2.59                     | 0.41              |
| 20:CT:44:LYS:HB3  | 20:CT:87:ALA:HB1  | 2.02                     | 0.41              |
| 50:D2:24:THR:HG23 | 50:D2:27:GLY:HA3  | 2.03                     | 0.41              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 22:DA:1096:A:C5    | 22:DA:1097:U:H5   | 2.39                     | 0.41              |
| 22:DA:116:C:C4     | 22:DA:117:G:N7    | 2.88                     | 0.41              |
| 22:DA:1275:A:C5    | 35:DN:16:HIS:CD2  | 3.08                     | 0.41              |
| 22:DA:128:C:C4     | 22:DA:129:C:N4    | 2.89                     | 0.41              |
| 22:DA:1358:G:O6    | 22:DA:1371:G:C8   | 2.74                     | 0.41              |
| 22:DA:1838:C:C4    | 22:DA:1899:A:C4   | 3.08                     | 0.41              |
| 22:DA:1877:A:H2'   | 22:DA:1878:G:C8   | 2.56                     | 0.41              |
| 22:DA:1911:U:H2'   | 22:DA:1918:A:C2   | 2.55                     | 0.41              |
| 22:DA:191:A:C2     | 22:DA:192:C:N3    | 2.89                     | 0.41              |
| 22:DA:2115:G:N3    | 22:DA:2117:A:C8   | 2.89                     | 0.41              |
| 22:DA:2134:A:C6    | 22:DA:2135:A:C5   | 3.08                     | 0.41              |
| 22:DA:2466:C:O2'   | 22:DA:2467:C:H5'  | 2.21                     | 0.41              |
| 22:DA:2516:A:C2'   | 22:DA:2517:C:O5'  | 2.69                     | 0.41              |
| 22:DA:2634:A:O2'   | 25:DD:79:LEU:HD12 | 2.21                     | 0.41              |
| 22:DA:2771:C:H2'   | 22:DA:2772:C:C6   | 2.55                     | 0.41              |
| 22:DA:373:U:C2     | 22:DA:374:A:C8    | 3.08                     | 0.41              |
| 22:DA:410:G:C6     | 22:DA:2407:A:N6   | 2.89                     | 0.41              |
| 22:DA:36:G:N2      | 22:DA:445:C:C2    | 2.89                     | 0.41              |
| 22:DA:513:A:C2     | 22:DA:514:A:N7    | 2.89                     | 0.41              |
| 22:DA:515:A:C8     | 22:DA:516:C:C6    | 3.08                     | 0.41              |
| 23:DB:15:A:H1'     | 23:DB:109:A:C8    | 2.56                     | 0.41              |
| 23:DB:90:C:C5'     | 34:DM:18:ARG:HG2  | 2.50                     | 0.41              |
| 24:DC:71:LYS:HG2   | 24:DC:102:ARG:CZ  | 2.51                     | 0.41              |
| 24:DC:252:THR:O    | 24:DC:253:LYS:HB2 | 2.21                     | 0.41              |
| 25:DD:8:LYS:HB2    | 25:DD:201:LEU:CD1 | 2.51                     | 0.41              |
| 26:DE:150:THR:O    | 26:DE:192:ALA:HB2 | 2.20                     | 0.41              |
| 27:DF:136:ILE:HG22 | 27:DF:136:ILE:O   | 2.21                     | 0.41              |
| 28:DG:62:TRP:HA    | 28:DG:62:TRP:CE3  | 2.56                     | 0.41              |
| 40:DS:47:VAL:O     | 40:DS:47:VAL:CG2  | 2.69                     | 0.41              |
| 41:DT:24:MET:CG    | 41:DT:29:THR:O    | 2.69                     | 0.41              |
| 42:DU:18:ASP:HB3   | 42:DU:21:LYS:HG3  | 2.01                     | 0.41              |
| 45:DX:54:LYS:HA    | 45:DX:57:ARG:CG   | 2.50                     | 0.41              |
| 1:AA:1080:A:OP1    | 5:AE:52:LYS:CE    | 2.68                     | 0.41              |
| 1:AA:1154:G:H2'    | 1:AA:1155:A:H8    | 1.86                     | 0.41              |
| 1:AA:960:U:H2'     | 1:AA:1225:A:H62   | 1.85                     | 0.41              |
| 1:AA:1323:G:O2'    | 1:AA:1324:A:H5'   | 2.21                     | 0.41              |
| 1:AA:1340:A:H2'    | 1:AA:1341:U:O4'   | 2.21                     | 0.41              |
| 1:AA:1401:G:C2     | 1:AA:1402:C:H1'   | 2.56                     | 0.41              |
| 1:AA:1461:G:H2'    | 1:AA:1462:C:H6    | 1.86                     | 0.41              |
| 1:AA:225:C:H2'     | 1:AA:226:G:O4'    | 2.20                     | 0.41              |
| 1:AA:591:U:H2'     | 1:AA:592:G:C8     | 2.56                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AA:737:C:C2     | 1:AA:738:C:C5     | 3.08                     | 0.41              |
| 1:AA:771:G:C5     | 1:AA:772:U:C5     | 3.08                     | 0.41              |
| 1:AA:865:A:H5'    | 1:AA:1078:U:O4    | 2.20                     | 0.41              |
| 2:AB:68:LEU:HD12  | 2:AB:154:MET:HE1  | 2.02                     | 0.41              |
| 3:AC:22:TRP:CD1   | 3:AC:59:ARG:HD2   | 2.56                     | 0.41              |
| 4:AD:28:ILE:HG22  | 4:AD:28:ILE:O     | 2.20                     | 0.41              |
| 5:AE:107:ALA:CB   | 5:AE:125:ALA:HB3  | 2.51                     | 0.41              |
| 5:AE:154:ALA:O    | 5:AE:157:ARG:C    | 2.59                     | 0.41              |
| 7:AG:108:ALA:O    | 7:AG:119:ARG:HD3  | 2.19                     | 0.41              |
| 7:AG:69:VAL:HG21  | 7:AG:104:ILE:CD1  | 2.50                     | 0.41              |
| 8:AH:41:LYS:O     | 8:AH:42:GLU:C     | 2.59                     | 0.41              |
| 9:AI:44:ALA:HB1   | 9:AI:47:VAL:CG1   | 2.50                     | 0.41              |
| 11:AK:31:ILE:O    | 11:AK:31:ILE:HG13 | 2.18                     | 0.41              |
| 13:AM:66:GLU:O    | 13:AM:69:LEU:N    | 2.54                     | 0.41              |
| 13:AM:8:ASN:OD1   | 13:AM:9:ILE:N     | 2.54                     | 0.41              |
| 16:AP:60:TRP:HA   | 16:AP:63:GLN:HB3  | 2.03                     | 0.41              |
| 16:AP:78:VAL:CG1  | 16:AP:78:VAL:O    | 2.68                     | 0.41              |
| 20:AT:67:ILE:HD12 | 20:AT:71:LYS:HG2  | 2.01                     | 0.41              |
| 53:B5:94:TYR:O    | 53:B5:95:VAL:HG23 | 2.20                     | 0.41              |
| 22:BA:1071:G:C4   | 22:BA:1089:A:C6   | 3.08                     | 0.41              |
| 22:BA:1106:G:C2   | 22:BA:1107:G:N9   | 2.88                     | 0.41              |
| 22:BA:1142:A:N3   | 22:BA:1144:A:C8   | 2.89                     | 0.41              |
| 22:BA:1301:A:N3   | 22:BA:1301:A:H2'  | 2.36                     | 0.41              |
| 22:BA:1346:G:C2'  | 22:BA:1347:A:H5'  | 2.51                     | 0.41              |
| 22:BA:1354:A:H2'  | 22:BA:1355:G:O4'  | 2.21                     | 0.41              |
| 22:BA:1421:G:H2'  | 22:BA:1421:G:N3   | 2.35                     | 0.41              |
| 22:BA:1441:G:H2'  | 22:BA:1442:U:H6   | 1.84                     | 0.41              |
| 22:BA:1452:G:C4   | 22:BA:2702:G:C6   | 3.09                     | 0.41              |
| 22:BA:167:A:H2'   | 22:BA:168:G:O4'   | 2.21                     | 0.41              |
| 22:BA:1906:G:C5   | 22:BA:1929:G:N2   | 2.88                     | 0.41              |
| 22:BA:2001:C:H4'  | 22:BA:2689:U:H2'  | 2.03                     | 0.41              |
| 22:BA:215:G:H4'   | 22:BA:216:A:OP1   | 2.20                     | 0.41              |
| 22:BA:2317:A:H2'  | 22:BA:2318:G:H5'  | 2.03                     | 0.41              |
| 22:BA:2486:C:H2'  | 22:BA:2487:G:O5'  | 2.19                     | 0.41              |
| 22:BA:2839:G:H2'  | 22:BA:2840:C:O5'  | 2.20                     | 0.41              |
| 22:BA:28:A:C5     | 22:BA:29:U:C5     | 3.08                     | 0.41              |
| 22:BA:416:U:H2'   | 22:BA:417:C:C6    | 2.55                     | 0.41              |
| 22:BA:770:G:O2'   | 22:BA:771:G:H5'   | 2.21                     | 0.41              |
| 22:BA:817:C:H2'   | 22:BA:818:G:O4'   | 2.21                     | 0.41              |
| 22:BA:971:G:C6    | 22:BA:972:A:C4    | 3.08                     | 0.41              |
| 24:BC:252:THR:O   | 24:BC:254:GLY:N   | 2.54                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 27:BF:17:MET:HE1  | 27:BF:22:TYR:HB2   | 2.01                     | 0.41              |
| 29:BH:129:GLU:C   | 29:BH:130:VAL:HG23 | 2.41                     | 0.41              |
| 29:BH:90:LEU:HG   | 29:BH:92:GLY:C     | 2.41                     | 0.41              |
| 31:BJ:23:LYS:CE   | 31:BJ:142:ILE:OXT  | 2.69                     | 0.41              |
| 34:BM:69:PRO:O    | 34:BM:70:ASP:OD2   | 2.39                     | 0.41              |
| 37:BP:110:ILE:O   | 37:BP:110:ILE:HG12 | 2.20                     | 0.41              |
| 39:BR:40:MET:O    | 39:BR:41:ILE:HG12  | 2.21                     | 0.41              |
| 42:BU:7:ARG:O     | 42:BU:8:ASP:O      | 2.38                     | 0.41              |
| 1:CA:1055:A:C5    | 1:CA:1206:G:C6     | 3.09                     | 0.41              |
| 1:CA:1090:U:H2'   | 1:CA:1091:U:C6     | 2.56                     | 0.41              |
| 1:CA:1092:A:C2    | 1:CA:1183:U:C2     | 3.09                     | 0.41              |
| 1:CA:1261:A:N6    | 1:CA:1275:A:N9     | 2.68                     | 0.41              |
| 1:CA:1293:C:H2'   | 1:CA:1294:G:O4'    | 2.21                     | 0.41              |
| 1:CA:1428:A:N1    | 1:CA:1473:G:C6     | 2.89                     | 0.41              |
| 1:CA:228:A:H2'    | 1:CA:229:U:O4'     | 2.21                     | 0.41              |
| 1:CA:243:A:C2     | 1:CA:246:A:C8      | 3.08                     | 0.41              |
| 1:CA:49:U:O4      | 1:CA:365:U:H5      | 2.03                     | 0.41              |
| 1:CA:4:U:C2'      | 1:CA:4:U:O2        | 2.68                     | 0.41              |
| 1:CA:69:G:H5'     | 1:CA:70:U:OP1      | 2.20                     | 0.41              |
| 2:CB:94:HIS:CG    | 2:CB:95:ARG:NH2    | 2.89                     | 0.41              |
| 3:CC:50:ALA:O     | 3:CC:51:SER:HB2    | 2.21                     | 0.41              |
| 4:CD:152:GLN:N    | 4:CD:152:GLN:OE1   | 2.53                     | 0.41              |
| 6:AF:17:GLN:HG2   | 4:CD:189:SER:HB2   | 2.02                     | 0.41              |
| 4:CD:58:LYS:HG3   | 4:CD:59:GLN:N      | 2.36                     | 0.41              |
| 9:CI:71:GLY:O     | 9:CI:75:GLN:N      | 2.46                     | 0.41              |
| 1:CA:684:U:O2     | 11:CK:41:ALA:HB3   | 2.21                     | 0.41              |
| 12:CL:43:LYS:O    | 12:CL:44:LYS:O     | 2.39                     | 0.41              |
| 12:CL:72:HIS:O    | 12:CL:72:HIS:ND1   | 2.54                     | 0.41              |
| 15:CO:60:VAL:O    | 15:CO:63:ARG:HB3   | 2.20                     | 0.41              |
| 20:CT:39:ILE:HD11 | 20:CT:83:ILE:CG2   | 2.51                     | 0.41              |
| 22:DA:1014:A:C6   | 22:DA:1015:U:C4    | 3.09                     | 0.41              |
| 22:DA:55:G:C2     | 22:DA:116:C:C2     | 3.09                     | 0.41              |
| 22:DA:1404:C:C2'  | 22:DA:1405:U:O5'   | 2.68                     | 0.41              |
| 22:DA:1439:A:C8   | 22:DA:1440:U:C6    | 3.09                     | 0.41              |
| 22:DA:1806:C:C5   | 22:DA:1807:G:C8    | 3.08                     | 0.41              |
| 22:DA:2209:G:C2   | 22:DA:2216:G:N3    | 2.88                     | 0.41              |
| 22:DA:2246:G:H2'  | 22:DA:2247:A:O4'   | 2.21                     | 0.41              |
| 22:DA:2281:A:H2'  | 22:DA:2282:G:H5'   | 2.03                     | 0.41              |
| 22:DA:2415:G:C5   | 22:DA:2416:C:C4    | 3.08                     | 0.41              |
| 22:DA:2646:C:N3   | 22:DA:2675:A:C2    | 2.89                     | 0.41              |
| 22:DA:2720:U:C4   | 22:DA:2872:A:C2    | 3.08                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:DA:2766:A:H2'  | 22:DA:2766:A:N3   | 2.36                     | 0.41              |
| 22:DA:2884:U:O4'  | 22:DA:2884:U:O2   | 2.38                     | 0.41              |
| 22:DA:291:G:N2    | 22:DA:350:G:C8    | 2.89                     | 0.41              |
| 22:DA:36:G:C2     | 22:DA:445:C:N3    | 2.88                     | 0.41              |
| 22:DA:377:G:C6    | 22:DA:378:C:N4    | 2.89                     | 0.41              |
| 22:DA:459:U:C5    | 22:DA:469:G:N2    | 2.88                     | 0.41              |
| 22:DA:565:C:C2'   | 22:DA:566:U:H5'   | 2.51                     | 0.41              |
| 22:DA:569:U:H2'   | 22:DA:570:G:O4'   | 2.21                     | 0.41              |
| 22:DA:688:U:OP1   | 50:D2:2:LYS:HD3   | 2.20                     | 0.41              |
| 22:DA:877:A:C2'   | 22:DA:878:A:OP2   | 2.68                     | 0.41              |
| 22:DA:952:G:C2    | 22:DA:966:G:C2    | 3.09                     | 0.41              |
| 23:DB:24:G:H4'    | 23:DB:25:U:C5     | 2.55                     | 0.41              |
| 26:DE:195:GLN:O   | 26:DE:199:MET:HB2 | 2.20                     | 0.41              |
| 26:DE:22:ASP:OD2  | 26:DE:22:ASP:N    | 2.54                     | 0.41              |
| 27:DF:69:LYS:HG3  | 27:DF:84:PRO:HA   | 2.02                     | 0.41              |
| 29:DH:118:PRO:HB2 | 29:DH:119:ASN:H   | 1.72                     | 0.41              |
| 29:DH:1:MET:HB3   | 29:DH:21:VAL:O    | 2.20                     | 0.41              |
| 29:DH:2:GLN:O     | 29:DH:3:VAL:O     | 2.38                     | 0.41              |
| 22:DA:1203:U:C1'  | 33:DL:4:ASN:HB3   | 2.47                     | 0.41              |
| 1:CA:345:C:OP1    | 37:DP:39:ARG:CD   | 2.69                     | 0.41              |
| 40:DS:33:LEU:CD2  | 40:DS:52:GLU:CG   | 2.98                     | 0.41              |
| 40:DS:57:ASN:N    | 40:DS:57:ASN:OD1  | 2.53                     | 0.41              |
| 22:DA:1599:U:P    | 41:DT:40:LYS:HD2  | 2.60                     | 0.41              |
| 43:DV:30:ILE:O    | 43:DV:37:PRO:HA   | 2.21                     | 0.41              |
| 44:DW:85:GLU:OE2  | 44:DW:85:GLU:HA   | 2.21                     | 0.41              |
| 46:DY:27:ASN:O    | 46:DY:31:GLN:HB2  | 2.21                     | 0.41              |
| 47:DZ:3:LYS:HD3   | 47:DZ:3:LYS:N     | 2.35                     | 0.41              |
| 1:AA:1059:C:N3    | 1:AA:1060:U:C5    | 2.89                     | 0.41              |
| 1:AA:1101:A:N3    | 1:AA:1102:A:H1'   | 2.36                     | 0.41              |
| 1:AA:1153:G:C4    | 1:AA:1154:G:C8    | 3.09                     | 0.41              |
| 1:AA:1258:G:O2'   | 1:AA:1259:C:H5'   | 2.21                     | 0.41              |
| 1:AA:1296:C:H5''  | 1:AA:1297:G:OP2   | 2.21                     | 0.41              |
| 1:AA:1239:A:H2'   | 1:AA:1298:U:O4    | 2.21                     | 0.41              |
| 1:AA:1412:C:H2'   | 1:AA:1413:A:C8    | 2.56                     | 0.41              |
| 1:AA:178:C:H2'    | 1:AA:179:A:O4'    | 2.21                     | 0.41              |
| 1:AA:181:A:N6     | 1:AA:195:A:C8     | 2.89                     | 0.41              |
| 1:AA:257:G:N2     | 1:AA:258:G:C4     | 2.89                     | 0.41              |
| 1:AA:375:U:C2     | 1:AA:376:G:C8     | 3.09                     | 0.41              |
| 1:AA:454:G:H2'    | 1:AA:455:G:H5'    | 2.02                     | 0.41              |
| 1:AA:539:A:H2'    | 1:AA:540:G:C8     | 2.56                     | 0.41              |
| 1:AA:615:G:C2     | 1:AA:616:G:C8     | 3.09                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AA:616:G:O2'    | 1:AA:617:G:H5'    | 2.20                     | 0.41              |
| 1:AA:697:U:C5     | 1:AA:698:G:C8     | 3.09                     | 0.41              |
| 1:AA:69:G:H3'     | 1:AA:70:U:C6      | 2.56                     | 0.41              |
| 2:AB:111:ILE:O    | 2:AB:114:LEU:N    | 2.54                     | 0.41              |
| 3:AC:97:VAL:HB    | 3:AC:98:PRO:HD2   | 2.02                     | 0.41              |
| 4:AD:97:ARG:O     | 4:AD:100:ASN:HB3  | 2.20                     | 0.41              |
| 4:AD:30:THR:O     | 4:AD:31:LYS:C     | 2.58                     | 0.41              |
| 8:AH:11:LEU:N     | 8:AH:11:LEU:HD23  | 2.36                     | 0.41              |
| 10:AJ:42:LEU:HG   | 10:AJ:43:PRO:HD2  | 2.02                     | 0.41              |
| 1:AA:728:A:OP1    | 15:AO:54:ARG:NH2  | 2.53                     | 0.41              |
| 16:AP:46:LYS:HD3  | 16:AP:47:GLU:H    | 1.82                     | 0.41              |
| 49:B1:25:LYS:CD   | 49:B1:52:ALA:O    | 2.69                     | 0.41              |
| 22:BA:71:A:N1     | 22:BA:114:U:H1'   | 2.36                     | 0.41              |
| 22:BA:218:A:OP2   | 57:BA:3225:HOH:O  | 2.22                     | 0.41              |
| 22:BA:2311:A:C8   | 27:BF:77:PHE:CG   | 3.08                     | 0.41              |
| 22:BA:2326:C:C1'  | 22:BA:2327:A:OP1  | 2.68                     | 0.41              |
| 22:BA:2331:G:O2'  | 22:BA:2336:A:N1   | 2.49                     | 0.41              |
| 22:BA:259:G:O2'   | 22:BA:260:G:H5'   | 2.20                     | 0.41              |
| 22:BA:2673:G:N3   | 22:BA:2674:G:C8   | 2.89                     | 0.41              |
| 22:BA:45:G:H5''   | 22:BA:46:G:OP1    | 2.21                     | 0.41              |
| 22:BA:523:C:C2'   | 22:BA:524:G:H5'   | 2.51                     | 0.41              |
| 22:BA:585:G:H5''  | 22:BA:586:A:OP1   | 2.21                     | 0.41              |
| 24:BC:221:ARG:NH2 | 57:BC:404:HOH:O   | 2.53                     | 0.41              |
| 22:BA:1816:C:C5   | 24:BC:62:TYR:CE1  | 3.09                     | 0.41              |
| 25:BD:11:MET:O    | 25:BD:12:THR:CG2  | 2.68                     | 0.41              |
| 32:BK:41:ILE:HD11 | 32:BK:58:LEU:HD22 | 2.02                     | 0.41              |
| 33:BL:81:ASP:HB3  | 33:BL:100:ILE:CD1 | 2.51                     | 0.41              |
| 22:BA:954:G:OP2   | 34:BM:16:ARG:NH2  | 2.54                     | 0.41              |
| 1:CA:109:A:N1     | 1:CA:327:A:C6     | 2.88                     | 0.41              |
| 1:CA:1183:U:C2'   | 1:CA:1184:G:OP1   | 2.69                     | 0.41              |
| 1:CA:1219:A:C6    | 1:CA:1220:G:C6    | 3.09                     | 0.41              |
| 1:CA:1327:C:N4    | 1:CA:1328:C:N4    | 2.68                     | 0.41              |
| 1:CA:1412:C:C2    | 1:CA:1413:A:C8    | 3.09                     | 0.41              |
| 1:CA:186:C:O2     | 1:CA:186:C:H2'    | 2.21                     | 0.41              |
| 1:CA:243:A:C2     | 1:CA:245:U:C2     | 3.09                     | 0.41              |
| 1:CA:463:U:H5'    | 1:CA:464:U:OP2    | 2.21                     | 0.41              |
| 1:CA:671:G:O2'    | 1:CA:672:U:H5'    | 2.21                     | 0.41              |
| 1:CA:867:G:C5     | 1:CA:868:C:C5     | 3.08                     | 0.41              |
| 1:CA:929:G:C5     | 1:CA:930:C:C5     | 3.08                     | 0.41              |
| 1:CA:976:G:C8     | 1:CA:1361:G:O6    | 2.74                     | 0.41              |
| 3:CC:134:MET:SD   | 3:CC:153:VAL:HG12 | 2.60                     | 0.41              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 3:CC:13:GLY:C     | 3:CC:14:ILE:HD13   | 2.41                     | 0.41              |
| 3:CC:167:TRP:C    | 3:CC:167:TRP:CE3   | 2.94                     | 0.41              |
| 3:CC:64:ILE:HG23  | 3:CC:99:ALA:HB2    | 2.02                     | 0.41              |
| 5:CE:156:LYS:HD3  | 8:CH:71:VAL:HG13   | 2.03                     | 0.41              |
| 6:CF:88:MET:SD    | 6:CF:90:MET:SD     | 3.19                     | 0.41              |
| 3:CC:23:PHE:CD2   | 10:CJ:97:ASP:HB2   | 2.56                     | 0.41              |
| 12:CL:38:TYR:O    | 12:CL:39:THR:HG23  | 2.21                     | 0.41              |
| 13:CM:22:ILE:HB   | 13:CM:25:VAL:CG1   | 2.51                     | 0.41              |
| 13:CM:34:LEU:HD22 | 13:CM:39:ILE:HG21  | 2.02                     | 0.41              |
| 15:CO:41:GLY:O    | 15:CO:42:HIS:C     | 2.59                     | 0.41              |
| 16:CP:28:ARG:CG   | 16:CP:29:ASN:N     | 2.84                     | 0.41              |
| 16:CP:4:ILE:CD1   | 16:CP:65:ALA:HB1   | 2.51                     | 0.41              |
| 21:CU:15:ALA:O    | 21:CU:16:LEU:C     | 2.59                     | 0.41              |
| 21:CU:4:ILE:N     | 21:CU:19:PHE:CE1   | 2.89                     | 0.41              |
| 22:DA:100:U:O4'   | 22:DA:101:A:C2     | 2.73                     | 0.41              |
| 22:DA:83:A:H2     | 22:DA:103:A:N7     | 2.18                     | 0.41              |
| 22:DA:116:C:C2    | 22:DA:117:G:C8     | 3.09                     | 0.41              |
| 22:DA:1237:A:N3   | 22:DA:1238:G:H1'   | 2.35                     | 0.41              |
| 22:DA:1483:G:C6   | 22:DA:1484:U:C4    | 3.09                     | 0.41              |
| 22:DA:1501:G:H2'  | 22:DA:1502:A:O4'   | 2.21                     | 0.41              |
| 22:DA:1844:C:C2   | 22:DA:1845:G:C8    | 3.09                     | 0.41              |
| 22:DA:1933:G:O2'  | 22:DA:1974:C:H4'   | 2.20                     | 0.41              |
| 22:DA:2127:G:O2'  | 22:DA:2173:A:C4    | 2.73                     | 0.41              |
| 22:DA:2503:A:C5'  | 22:DA:2503:A:N3    | 2.84                     | 0.41              |
| 22:DA:2553:G:H2'  | 22:DA:2554:U:C4'   | 2.50                     | 0.41              |
| 22:DA:404:A:C1'   | 22:DA:405:U:OP2    | 2.69                     | 0.41              |
| 22:DA:420:C:H2'   | 22:DA:421:C:H6     | 1.85                     | 0.41              |
| 22:DA:826:U:H5''  | 57:DA:3696:HOH:O   | 2.19                     | 0.41              |
| 24:DC:53:HIS:HA   | 24:DC:217:ARG:HB2  | 2.03                     | 0.41              |
| 26:DE:135:ALA:O   | 26:DE:139:LYS:HB2  | 2.20                     | 0.41              |
| 27:DF:99:PHE:HA   | 27:DF:102:ARG:NE   | 2.36                     | 0.41              |
| 27:DF:9:LYS:O     | 27:DF:13:VAL:HB    | 2.21                     | 0.41              |
| 30:DI:22:PRO:CB   | 30:DI:23:PRO:HD3   | 2.51                     | 0.41              |
| 31:DJ:4:PHE:CG    | 38:DQ:100:VAL:HG11 | 2.56                     | 0.41              |
| 34:DM:34:LYS:O    | 34:DM:128:THR:CG2  | 2.68                     | 0.41              |
| 22:DA:869:G:H1'   | 34:DM:8:LYS:HD2    | 2.01                     | 0.41              |
| 36:DO:97:PHE:HB3  | 36:DO:103:VAL:HG11 | 2.01                     | 0.41              |
| 32:DK:78:ARG:NH2  | 37:DP:73:VAL:CG1   | 2.84                     | 0.41              |
| 38:DQ:25:TYR:CD2  | 38:DQ:25:TYR:C     | 2.94                     | 0.41              |
| 38:DQ:58:ARG:NH2  | 38:DQ:92:ARG:CZ    | 2.84                     | 0.41              |
| 40:DS:58:ALA:O    | 40:DS:62:ASP:O     | 2.39                     | 0.41              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:AA:1130:A:C2    | 1:AA:1146:A:C4    | 3.09                     | 0.41              |
| 1:AA:1288:A:C6    | 1:AA:1289:A:C5    | 3.08                     | 0.41              |
| 1:AA:258:G:C5     | 1:AA:259:G:N7     | 2.89                     | 0.41              |
| 1:AA:451:A:H4'    | 1:AA:452:A:O5'    | 2.21                     | 0.41              |
| 1:AA:459:A:H2'    | 1:AA:460:A:C8     | 2.56                     | 0.41              |
| 1:AA:669:G:O2'    | 1:AA:670:G:H5'    | 2.21                     | 0.41              |
| 1:AA:704:A:C6     | 1:AA:705:G:C4     | 3.09                     | 0.41              |
| 1:AA:953:G:C2     | 1:AA:1229:A:C2    | 3.09                     | 0.41              |
| 1:AA:958:A:N6     | 1:AA:959:A:N1     | 2.69                     | 0.41              |
| 1:AA:987:G:H2'    | 1:AA:987:G:N3     | 2.36                     | 0.41              |
| 2:AB:101:LEU:HD13 | 2:AB:101:LEU:HA   | 1.90                     | 0.41              |
| 2:AB:149:GLY:O    | 2:AB:152:LYS:N    | 2.53                     | 0.41              |
| 2:AB:79:ALA:C     | 2:AB:82:ASP:OD2   | 2.58                     | 0.41              |
| 9:AI:29:VAL:HB    | 9:AI:64:TYR:HA    | 2.03                     | 0.41              |
| 11:AK:55:SER:O    | 11:AK:56:ARG:C    | 2.58                     | 0.41              |
| 11:AK:82:LEU:O    | 11:AK:82:LEU:HD23 | 2.20                     | 0.41              |
| 13:AM:29:ARG:CZ   | 13:AM:63:PHE:CB   | 2.99                     | 0.41              |
| 19:AS:4:SER:O     | 19:AS:5:LEU:HB2   | 2.21                     | 0.41              |
| 19:AS:50:ALA:HB1  | 19:AS:57:HIS:CB   | 2.51                     | 0.41              |
| 20:AT:43:ASP:O    | 20:AT:47:ALA:HB2  | 2.21                     | 0.41              |
| 22:BA:1088:A:N3   | 22:BA:1088:A:H3'  | 2.36                     | 0.41              |
| 22:BA:1121:C:H2'  | 22:BA:1122:G:O4'  | 2.22                     | 0.41              |
| 22:BA:1014:A:C2   | 22:BA:1149:G:C4   | 3.08                     | 0.41              |
| 22:BA:1153:C:C4   | 22:BA:1154:G:C5   | 3.09                     | 0.41              |
| 22:BA:1165:A:H2'  | 22:BA:1166:G:H8   | 1.86                     | 0.41              |
| 22:BA:2127:G:H5'  | 22:BA:2128:G:OP1  | 2.21                     | 0.41              |
| 22:BA:2188:U:C4   | 22:BA:2189:U:O4   | 2.74                     | 0.41              |
| 22:BA:21:A:O2'    | 22:BA:22:C:H5'    | 2.21                     | 0.41              |
| 22:BA:2516:A:N6   | 22:BA:2517:C:N4   | 2.68                     | 0.41              |
| 22:BA:300:A:OP2   | 42:BU:97:LYS:NZ   | 2.53                     | 0.41              |
| 22:BA:49:A:C8     | 22:BA:51:G:C2     | 3.09                     | 0.41              |
| 22:BA:597:G:C6    | 22:BA:598:U:C4    | 3.08                     | 0.41              |
| 22:BA:790:U:HO2'  | 22:BA:791:C:P     | 2.43                     | 0.41              |
| 23:BB:28:C:OP1    | 36:BO:31:THR:HG21 | 2.20                     | 0.41              |
| 23:BB:35:C:C3'    | 23:BB:36:C:H5'    | 2.50                     | 0.41              |
| 22:BA:764:A:OP2   | 24:BC:213:TRP:CZ3 | 2.74                     | 0.41              |
| 24:BC:36:LYS:O    | 24:BC:37:ASN:HB3  | 2.19                     | 0.41              |
| 26:BE:25:GLU:O    | 26:BE:26:ALA:C    | 2.59                     | 0.41              |
| 27:BF:119:ALA:HB1 | 27:BF:167:ARG:CD  | 2.51                     | 0.41              |
| 27:BF:33:LYS:HG2  | 27:BF:157:THR:HB  | 2.02                     | 0.41              |
| 29:BH:129:GLU:C   | 29:BH:130:VAL:CG2 | 2.90                     | 0.41              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 29:BH:132:PHE:CE2  | 29:BH:142:VAL:CG2 | 3.04                     | 0.41              |
| 30:BI:115:ALA:O    | 30:BI:116:ASP:HB2 | 2.21                     | 0.41              |
| 30:BI:122:ILE:HG23 | 30:BI:125:MET:SD  | 2.61                     | 0.41              |
| 30:BI:33:VAL:HG13  | 30:BI:67:PHE:CZ   | 2.56                     | 0.41              |
| 31:BJ:7:LYS:HA     | 31:BJ:8:PRO:HD3   | 1.85                     | 0.41              |
| 33:BL:85:VAL:HA    | 33:BL:98:ALA:HB2  | 2.02                     | 0.41              |
| 34:BM:135:VAL:O    | 34:BM:136:MET:HB3 | 2.21                     | 0.41              |
| 35:BN:38:LEU:N     | 35:BN:39:PRO:CD   | 2.84                     | 0.41              |
| 35:BN:9:GLN:O      | 35:BN:11:ASN:N    | 2.54                     | 0.41              |
| 38:BQ:81:ASN:O     | 38:BQ:84:LYS:HB3  | 2.21                     | 0.41              |
| 39:BR:11:GLN:C     | 39:BR:12:HIS:CG   | 2.94                     | 0.41              |
| 40:BS:29:VAL:CG1   | 40:BS:55:ILE:CD1  | 2.99                     | 0.41              |
| 41:BT:61:LEU:HD12  | 41:BT:61:LEU:C    | 2.42                     | 0.41              |
| 41:BT:69:ARG:CB    | 41:BT:74:ILE:HG22 | 2.50                     | 0.41              |
| 1:CA:1072:G:C4     | 1:CA:1104:G:N2    | 2.89                     | 0.41              |
| 1:CA:1263:C:C5     | 1:CA:1264:U:C5    | 3.09                     | 0.41              |
| 1:CA:1502:A:C8     | 1:CA:1504:G:C4    | 3.09                     | 0.41              |
| 1:CA:263:A:P       | 20:CT:74:ARG:NH1  | 2.94                     | 0.41              |
| 1:CA:748:G:C2      | 1:CA:749:A:C5     | 3.09                     | 0.41              |
| 1:CA:74:A:C2       | 1:CA:75:G:C8      | 3.09                     | 0.41              |
| 1:CA:77:A:C2       | 1:CA:93:U:N3      | 2.89                     | 0.41              |
| 1:CA:822:U:C2      | 1:CA:823:C:C5     | 3.08                     | 0.41              |
| 1:CA:9:G:C2        | 1:CA:10:A:C8      | 3.08                     | 0.41              |
| 2:CB:102:THR:HA    | 2:CB:179:LEU:HD21 | 2.01                     | 0.41              |
| 2:CB:199:VAL:C     | 2:CB:200:ILE:HD12 | 2.41                     | 0.41              |
| 2:CB:207:ILE:O     | 2:CB:210:VAL:HG13 | 2.21                     | 0.41              |
| 5:CE:83:HIS:HB2    | 5:CE:84:PRO:HD2   | 2.01                     | 0.41              |
| 6:CF:51:ILE:HG12   | 6:CF:51:ILE:O     | 2.21                     | 0.41              |
| 6:CF:70:VAL:HG23   | 6:CF:71:ILE:HD12  | 2.01                     | 0.41              |
| 7:CG:71:PRO:HD2    | 7:CG:96:ARG:HG2   | 2.03                     | 0.41              |
| 11:CK:36:ASP:CG    | 11:CK:40:ASN:HB2  | 2.42                     | 0.41              |
| 16:CP:39:PHE:O     | 16:CP:41:PRO:HD3  | 2.21                     | 0.41              |
| 17:CQ:52:GLU:CD    | 17:CQ:75:LEU:HD21 | 2.42                     | 0.41              |
| 22:DA:2370:G:H4'   | 49:D1:44:ARG:NH1  | 2.35                     | 0.41              |
| 22:DA:1059:G:N2    | 30:DI:131:GLY:HA3 | 2.36                     | 0.41              |
| 22:DA:1469:A:C2    | 22:DA:1470:A:C5   | 3.09                     | 0.41              |
| 22:DA:178:G:C6     | 22:DA:179:C:C5    | 3.09                     | 0.41              |
| 22:DA:1838:C:C5    | 22:DA:1899:A:C6   | 3.09                     | 0.41              |
| 22:DA:206:U:C2     | 22:DA:207:A:C8    | 3.08                     | 0.41              |
| 22:DA:2125:G:H5'   | 22:DA:2126:A:OP2  | 2.21                     | 0.41              |
| 22:DA:2282:G:OP1   | 22:DA:2283:C:H1'  | 2.21                     | 0.41              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 22:DA:2420:C:OP1   | 51:D3:34:THR:CB   | 2.68                     | 0.41              |
| 22:DA:2728:U:O2'   | 22:DA:2729:G:H5'' | 2.21                     | 0.41              |
| 22:DA:2819:G:H1'   | 22:DA:2828:G:N2   | 2.36                     | 0.41              |
| 22:DA:283:G:C5     | 22:DA:284:U:C5    | 3.09                     | 0.41              |
| 22:DA:396:G:H5'    | 22:DA:396:G:H8    | 1.86                     | 0.41              |
| 22:DA:802:A:H2'    | 22:DA:803:U:C6    | 2.56                     | 0.41              |
| 22:DA:79:C:C4      | 22:DA:80:G:N7     | 2.89                     | 0.41              |
| 23:DB:59:A:H2'     | 23:DB:60:C:O4'    | 2.20                     | 0.41              |
| 23:DB:67:G:C6      | 23:DB:68:C:N4     | 2.89                     | 0.41              |
| 28:DG:123:ALA:CB   | 28:DG:133:LEU:HA  | 2.50                     | 0.41              |
| 28:DG:24:ILE:CD1   | 28:DG:43:VAL:HG11 | 2.51                     | 0.41              |
| 28:DG:39:ASP:O     | 28:DG:58:TYR:CE1  | 2.74                     | 0.41              |
| 33:DL:111:ILE:HG22 | 33:DL:112:LEU:N   | 2.36                     | 0.41              |
| 34:DM:2:LEU:HB2    | 34:DM:69:PRO:HG2  | 2.03                     | 0.41              |
| 1:AA:1035:A:H2'    | 1:AA:1036:A:C1'   | 2.51                     | 0.40              |
| 1:AA:1058:G:C5     | 1:AA:1059:C:C5    | 3.10                     | 0.40              |
| 1:AA:1211:U:O2'    | 1:AA:1212:U:P     | 2.78                     | 0.40              |
| 1:AA:1385:G:O2'    | 1:AA:1386:G:H5'   | 2.21                     | 0.40              |
| 1:AA:146:G:C2      | 1:AA:147:G:C4     | 3.10                     | 0.40              |
| 1:AA:1533:C:C5'    | 1:AA:1534:A:OP1   | 2.70                     | 0.40              |
| 1:AA:223:A:H2'     | 1:AA:224:U:C6     | 2.56                     | 0.40              |
| 1:AA:270:A:H2'     | 1:AA:271:C:O4'    | 2.21                     | 0.40              |
| 1:AA:457:G:O6      | 1:AA:458:U:N3     | 2.54                     | 0.40              |
| 1:AA:774:G:C4      | 1:AA:775:G:C8     | 3.09                     | 0.40              |
| 1:AA:790:A:H2'     | 1:AA:791:G:C8     | 2.56                     | 0.40              |
| 1:AA:827:U:H2'     | 1:AA:870:U:O4     | 2.21                     | 0.40              |
| 1:AA:955:U:O4'     | 1:AA:1227:A:N6    | 2.52                     | 0.40              |
| 1:AA:987:G:H5'     | 1:AA:988:G:OP2    | 2.21                     | 0.40              |
| 2:AB:171:ILE:O     | 2:AB:175:GLU:HG3  | 2.21                     | 0.40              |
| 2:AB:186:ILE:HD11  | 2:AB:204:ASP:HA   | 2.02                     | 0.40              |
| 2:AB:62:SER:C      | 2:AB:64:LYS:N     | 2.74                     | 0.40              |
| 3:AC:10:ILE:HG13   | 3:AC:10:ILE:O     | 2.21                     | 0.40              |
| 3:AC:14:ILE:N      | 3:AC:14:ILE:HD13  | 2.36                     | 0.40              |
| 4:AD:4:TYR:CE2     | 4:AD:11:LEU:HD11  | 2.56                     | 0.40              |
| 4:AD:98:LEU:O      | 4:AD:99:ASP:C     | 2.59                     | 0.40              |
| 5:AE:151:GLU:C     | 5:AE:153:VAL:H    | 2.24                     | 0.40              |
| 11:AK:61:PHE:O     | 11:AK:64:GLN:N    | 2.54                     | 0.40              |
| 13:AM:77:ILE:O     | 13:AM:80:LEU:HB2  | 2.21                     | 0.40              |
| 14:AN:68:GLY:O     | 14:AN:69:ARG:C    | 2.58                     | 0.40              |
| 20:AT:35:VAL:HG11  | 20:AT:79:LEU:HD22 | 2.03                     | 0.40              |
| 22:BA:1014:A:C2    | 22:BA:1149:G:N3   | 2.89                     | 0.40              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:BA:1366:A:C5   | 22:BA:1367:A:C8    | 3.09                     | 0.40              |
| 22:BA:1577:C:H2'  | 22:BA:1578:U:O4'   | 2.21                     | 0.40              |
| 22:BA:1856:U:C4   | 22:BA:1857:G:C6    | 3.09                     | 0.40              |
| 22:BA:1936:A:C2   | 22:BA:1943:U:N3    | 2.87                     | 0.40              |
| 22:BA:2001:C:N3   | 22:BA:2002:G:C8    | 2.89                     | 0.40              |
| 22:BA:2190:G:C4   | 22:BA:2191:A:C8    | 3.09                     | 0.40              |
| 22:BA:2243:U:H2'  | 22:BA:2244:U:H6    | 1.85                     | 0.40              |
| 22:BA:2492:U:H2'  | 22:BA:2493:U:C6    | 2.55                     | 0.40              |
| 22:BA:2498:C:P    | 57:BA:3686:HOH:O   | 2.61                     | 0.40              |
| 22:BA:2615:U:H1'  | 48:B0:4:GLN:HB3    | 2.02                     | 0.40              |
| 22:BA:2690:U:C4   | 22:BA:2873:A:C2    | 3.09                     | 0.40              |
| 22:BA:328:U:H2'   | 22:BA:329:G:OP1    | 2.20                     | 0.40              |
| 22:BA:449:A:C6    | 22:BA:450:G:C5     | 3.09                     | 0.40              |
| 22:BA:451:U:H5'   | 57:BA:3238:HOH:O   | 2.21                     | 0.40              |
| 22:BA:958:U:H2'   | 23:BB:89:U:O2      | 2.22                     | 0.40              |
| 26:BE:157:LEU:HG  | 26:BE:169:VAL:HG21 | 2.02                     | 0.40              |
| 26:BE:4:VAL:C     | 26:BE:6:LYS:H      | 2.24                     | 0.40              |
| 27:BF:20:PHE:O    | 27:BF:21:ASN:C     | 2.59                     | 0.40              |
| 27:BF:44:ILE:HG21 | 27:BF:79:ILE:CG2   | 2.51                     | 0.40              |
| 29:BH:88:GLY:C    | 29:BH:125:THR:OG1  | 2.59                     | 0.40              |
| 31:BJ:31:GLU:OE1  | 31:BJ:34:ARG:NE    | 2.54                     | 0.40              |
| 35:BN:71:ARG:O    | 35:BN:71:ARG:CG    | 2.69                     | 0.40              |
| 37:BP:16:ASP:OD1  | 37:BP:16:ASP:C     | 2.59                     | 0.40              |
| 38:BQ:99:ALA:O    | 38:BQ:103:LYS:HE2  | 2.21                     | 0.40              |
| 41:BT:1:MET:HG3   | 41:BT:2:ILE:N      | 2.36                     | 0.40              |
| 1:CA:1049:U:OP1   | 57:CA:1846:HOH:O   | 2.21                     | 0.40              |
| 1:CA:1049:U:H4'   | 1:CA:1050:G:O5'    | 2.20                     | 0.40              |
| 1:CA:1244:G:H2'   | 1:CA:1245:C:C6     | 2.56                     | 0.40              |
| 1:CA:128:G:C2     | 1:CA:234:C:C2      | 3.09                     | 0.40              |
| 1:CA:189:A:N6     | 1:CA:190:A:C2      | 2.89                     | 0.40              |
| 1:CA:243:A:C5     | 1:CA:281:G:N2      | 2.90                     | 0.40              |
| 1:CA:263:A:OP1    | 20:CT:74:ARG:NH1   | 2.53                     | 0.40              |
| 1:CA:453:G:H2'    | 1:CA:454:G:C8      | 2.56                     | 0.40              |
| 1:CA:782:A:C5     | 1:CA:801:U:N3      | 2.89                     | 0.40              |
| 1:CA:793:U:HO2'   | 1:CA:1516:G:C1'    | 2.34                     | 0.40              |
| 1:CA:799:G:C6     | 1:CA:800:G:C4      | 3.09                     | 0.40              |
| 1:CA:923:A:H2'    | 1:CA:924:C:O4'     | 2.21                     | 0.40              |
| 1:CA:975:A:N3     | 1:CA:975:A:H5'     | 2.36                     | 0.40              |
| 2:CB:141:LEU:O    | 2:CB:143:LYS:N     | 2.54                     | 0.40              |
| 3:CC:154:SER:CB   | 3:CC:165:THR:HG22  | 2.51                     | 0.40              |
| 4:CD:194:ASP:O    | 4:CD:195:ILE:CG2   | 2.69                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 4:CD:9:LEU:HD13    | 4:CD:9:LEU:HA      | 1.80                     | 0.40              |
| 7:CG:136:LYS:O     | 7:CG:136:LYS:HD2   | 2.21                     | 0.40              |
| 8:CH:95:VAL:CG1    | 8:CH:96:MET:N      | 2.84                     | 0.40              |
| 9:CI:28:ILE:HG21   | 9:CI:35:LEU:HD22   | 2.02                     | 0.40              |
| 11:CK:124:PRO:HB2  | 11:CK:126:LYS:CD   | 2.50                     | 0.40              |
| 12:CL:114:ARG:CZ   | 12:CL:121:ARG:HA   | 2.51                     | 0.40              |
| 16:CP:19:VAL:CG1   | 16:CP:37:GLY:CA    | 2.99                     | 0.40              |
| 48:D0:43:ILE:HG22  | 48:D0:49:TYR:HB2   | 2.03                     | 0.40              |
| 49:D1:25:LYS:HE2   | 49:D1:30:LYS:O     | 2.20                     | 0.40              |
| 49:D1:40:ASP:HA    | 49:D1:41:PRO:HD2   | 1.90                     | 0.40              |
| 22:DA:1203:U:H1'   | 33:DL:4:ASN:CB     | 2.46                     | 0.40              |
| 22:DA:140:C:O2     | 22:DA:140:C:O4'    | 2.37                     | 0.40              |
| 22:DA:1436:G:N2    | 22:DA:1557:C:C2    | 2.89                     | 0.40              |
| 22:DA:176:A:C5     | 22:DA:177:G:C6     | 3.09                     | 0.40              |
| 22:DA:120:U:O4     | 22:DA:177:G:N7     | 2.54                     | 0.40              |
| 22:DA:1783:A:C5'   | 22:DA:2608:G:H4'   | 2.51                     | 0.40              |
| 22:DA:2128:G:C4    | 22:DA:2173:A:O2'   | 2.74                     | 0.40              |
| 22:DA:2322:A:N6    | 22:DA:2323:G:C6    | 2.89                     | 0.40              |
| 22:DA:2457:U:C4    | 22:DA:2458:G:C6    | 3.09                     | 0.40              |
| 22:DA:2820:A:C6    | 25:DD:197:THR:HB   | 2.56                     | 0.40              |
| 22:DA:2690:U:C5    | 22:DA:2873:A:N1    | 2.89                     | 0.40              |
| 22:DA:2896:C:C2'   | 22:DA:2897:U:O5'   | 2.69                     | 0.40              |
| 22:DA:319:G:N9     | 22:DA:333:G:N2     | 2.69                     | 0.40              |
| 22:DA:270:A:H2     | 22:DA:369:U:H4'    | 1.85                     | 0.40              |
| 22:DA:46:G:C2'     | 22:DA:47:C:O5'     | 2.69                     | 0.40              |
| 22:DA:647:G:C5     | 22:DA:648:G:C5     | 3.08                     | 0.40              |
| 22:DA:690:G:H1'    | 22:DA:779:U:O3'    | 2.21                     | 0.40              |
| 22:DA:779:U:H5''   | 24:DC:49:ILE:HD11  | 2.02                     | 0.40              |
| 22:DA:537:G:OP1    | 22:DA:995:C:N4     | 2.54                     | 0.40              |
| 23:DB:77:U:C2'     | 23:DB:78:A:H5'     | 2.50                     | 0.40              |
| 22:DA:1820:U:OP1   | 24:DC:177:ARG:HG3  | 2.21                     | 0.40              |
| 24:DC:192:LEU:N    | 24:DC:192:LEU:HD22 | 2.36                     | 0.40              |
| 25:DD:4:LEU:HD22   | 25:DD:101:PHE:CE2  | 2.56                     | 0.40              |
| 22:DA:2052:A:OP1   | 25:DD:146:ILE:HG12 | 2.21                     | 0.40              |
| 25:DD:186:LEU:HD21 | 37:DP:4:ILE:CG2    | 2.51                     | 0.40              |
| 27:DF:16:LEU:HD11  | 27:DF:169:LEU:HD12 | 2.03                     | 0.40              |
| 27:DF:117:LEU:CD2  | 27:DF:176:PRO:HG2  | 2.51                     | 0.40              |
| 22:DA:1059:G:H1'   | 30:DI:117:MET:HE1  | 2.02                     | 0.40              |
| 31:DJ:120:ARG:O    | 31:DJ:123:LYS:NZ   | 2.37                     | 0.40              |
| 33:DL:77:ILE:HG23  | 33:DL:81:ASP:OD2   | 2.21                     | 0.40              |
| 35:DN:103:ARG:HD3  | 35:DN:110:MET:SD   | 2.60                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 32:DK:121:GLU:OE2 | 37:DP:66:ASN:OD1  | 2.39                     | 0.40              |
| 37:DP:31:TRP:NE1  | 37:DP:82:ASP:OD1  | 2.54                     | 0.40              |
| 39:DR:67:GLY:C    | 39:DR:93:PHE:CE2  | 2.94                     | 0.40              |
| 42:DU:56:GLY:O    | 42:DU:57:GLY:C    | 2.59                     | 0.40              |
| 44:DW:67:VAL:HG12 | 44:DW:68:LYS:N    | 2.37                     | 0.40              |
| 1:AA:1210:C:C4    | 1:AA:1211:U:C4    | 3.09                     | 0.40              |
| 1:AA:1211:U:H1'   | 1:AA:1213:A:C2    | 2.56                     | 0.40              |
| 1:AA:1259:C:O2    | 1:AA:1283:U:H1'   | 2.21                     | 0.40              |
| 1:AA:1324:A:H2'   | 1:AA:1325:C:C6    | 2.56                     | 0.40              |
| 1:AA:147:G:H2'    | 1:AA:148:G:C8     | 2.56                     | 0.40              |
| 1:AA:457:G:C6     | 1:AA:458:U:C2     | 3.09                     | 0.40              |
| 1:AA:53:A:C2'     | 1:AA:54:C:O5'     | 2.70                     | 0.40              |
| 1:AA:862:C:H2'    | 1:AA:863:U:H5'    | 2.02                     | 0.40              |
| 1:AA:914:A:C6     | 1:AA:915:A:C5     | 3.09                     | 0.40              |
| 2:AB:144:LEU:O    | 2:AB:145:GLU:C    | 2.60                     | 0.40              |
| 2:AB:167:ASP:O    | 2:AB:170:HIS:ND1  | 2.55                     | 0.40              |
| 4:AD:147:GLU:O    | 4:AD:148:LYS:C    | 2.59                     | 0.40              |
| 4:AD:78:GLU:CG    | 4:AD:93:LEU:HD21  | 2.51                     | 0.40              |
| 10:AJ:65:TYR:HB3  | 14:AN:96:LEU:HD11 | 2.03                     | 0.40              |
| 10:AJ:8:ILE:O     | 10:AJ:73:LEU:O    | 2.39                     | 0.40              |
| 11:AK:65:VAL:O    | 11:AK:65:VAL:CG2  | 2.69                     | 0.40              |
| 12:AL:3:THR:HB    | 12:AL:6:GLN:HG3   | 2.03                     | 0.40              |
| 12:AL:72:HIS:ND1  | 12:AL:74:LEU:HB2  | 2.37                     | 0.40              |
| 12:AL:74:LEU:HD21 | 12:AL:104:CYS:HA  | 2.02                     | 0.40              |
| 16:AP:38:PHE:C    | 16:AP:38:PHE:CD1  | 2.94                     | 0.40              |
| 20:AT:15:GLU:OE1  | 20:AT:19:LYS:NZ   | 2.55                     | 0.40              |
| 20:AT:46:ALA:HA   | 20:AT:49:LYS:HB2  | 2.03                     | 0.40              |
| 53:B5:133:GLY:O   | 53:B5:134:PRO:CB  | 2.69                     | 0.40              |
| 53:B5:49:GLY:CA   | 53:B5:206:LYS:CB  | 2.99                     | 0.40              |
| 22:BA:1142:A:C4   | 22:BA:1144:A:C8   | 3.10                     | 0.40              |
| 22:BA:1671:U:O2   | 22:BA:1673:G:C8   | 2.75                     | 0.40              |
| 22:BA:1759:A:H2'  | 22:BA:1760:C:C6   | 2.55                     | 0.40              |
| 22:BA:1838:C:N4   | 22:BA:1899:A:C4   | 2.90                     | 0.40              |
| 22:BA:1844:C:C2   | 22:BA:1897:G:C2   | 3.10                     | 0.40              |
| 11:AK:69:ARG:HD2  | 22:BA:2146:C:C4   | 2.56                     | 0.40              |
| 22:BA:2176:A:H2'  | 22:BA:2177:C:C6   | 2.56                     | 0.40              |
| 22:BA:2345:G:N3   | 22:BA:2381:A:H2'  | 2.36                     | 0.40              |
| 22:BA:2564:A:C5   | 22:BA:2565:A:C6   | 3.10                     | 0.40              |
| 22:BA:2824:C:C4   | 22:BA:2825:G:C5   | 3.09                     | 0.40              |
| 22:BA:669:G:C2'   | 22:BA:669:G:N3    | 2.83                     | 0.40              |
| 22:BA:767:U:O2'   | 22:BA:768:G:H5'   | 2.21                     | 0.40              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 22:BA:839:U:H2'   | 22:BA:840:C:C6     | 2.56                     | 0.40              |
| 24:BC:247:PRO:HG2 | 24:BC:248:TRP:CZ3  | 2.56                     | 0.40              |
| 24:BC:97:LYS:HD2  | 24:BC:97:LYS:N     | 2.35                     | 0.40              |
| 26:BE:4:VAL:O     | 26:BE:4:VAL:HG22   | 2.21                     | 0.40              |
| 30:BI:116:ASP:O   | 30:BI:117:MET:CG   | 2.70                     | 0.40              |
| 31:BJ:37:ARG:O    | 31:BJ:37:ARG:HG3   | 2.21                     | 0.40              |
| 32:BK:102:PRO:HB3 | 32:BK:121:GLU:HB2  | 2.04                     | 0.40              |
| 35:BN:9:GLN:O     | 35:BN:10:LEU:C     | 2.60                     | 0.40              |
| 1:AA:1442:G:H5'   | 37:BP:114:LEU:HD13 | 2.04                     | 0.40              |
| 39:BR:49:ILE:HG13 | 39:BR:49:ILE:O     | 2.21                     | 0.40              |
| 42:BU:57:GLY:O    | 42:BU:59:VAL:HG23  | 2.21                     | 0.40              |
| 47:BZ:35:THR:CG2  | 47:BZ:36:VAL:N     | 2.84                     | 0.40              |
| 1:CA:1070:U:H2'   | 1:CA:1071:C:H6     | 1.86                     | 0.40              |
| 1:CA:1295:U:H2'   | 1:CA:1296:C:C6     | 2.56                     | 0.40              |
| 1:CA:1500:A:C5    | 1:CA:1501:C:C5     | 3.09                     | 0.40              |
| 1:CA:207:C:H2'    | 1:CA:207:C:O2      | 2.21                     | 0.40              |
| 1:CA:374:A:OP1    | 1:CA:452:A:N1      | 2.54                     | 0.40              |
| 1:CA:577:G:N3     | 1:CA:578:C:C6      | 2.90                     | 0.40              |
| 1:CA:599:C:C2     | 1:CA:640:A:C2      | 3.09                     | 0.40              |
| 1:CA:659:U:O2'    | 1:CA:660:C:H5'     | 2.21                     | 0.40              |
| 2:CB:139:ARG:HD2  | 2:CB:140:GLU:N     | 2.36                     | 0.40              |
| 4:CD:102:VAL:HG13 | 4:CD:107:PHE:HB2   | 2.04                     | 0.40              |
| 4:CD:30:THR:O     | 4:CD:31:LYS:HD3    | 2.21                     | 0.40              |
| 5:CE:147:MET:HG2  | 5:CE:147:MET:O     | 2.21                     | 0.40              |
| 7:CG:91:VAL:HG21  | 7:CG:96:ARG:HA     | 2.03                     | 0.40              |
| 17:CQ:38:ILE:HG22 | 17:CQ:39:LYS:O     | 2.21                     | 0.40              |
| 50:D2:6:GLN:HA    | 50:D2:6:GLN:OE1    | 2.21                     | 0.40              |
| 22:DA:2392:A:H4'  | 51:D3:28:ASN:OD1   | 2.22                     | 0.40              |
| 22:DA:2351:G:O6   | 51:D3:39:LYS:HE3   | 2.21                     | 0.40              |
| 22:DA:1090:A:C6   | 22:DA:1102:C:O2    | 2.74                     | 0.40              |
| 22:DA:1022:G:C5   | 22:DA:1140:C:C4    | 3.10                     | 0.40              |
| 22:DA:1378:A:O3'  | 57:DA:3751:HOH:O   | 2.21                     | 0.40              |
| 22:DA:145:C:H2'   | 22:DA:146:A:C8     | 2.56                     | 0.40              |
| 22:DA:1645:G:H5'' | 22:DA:1646:C:C5'   | 2.50                     | 0.40              |
| 22:DA:1989:G:C2'  | 22:DA:1990:C:H5'   | 2.51                     | 0.40              |
| 22:DA:200:U:C6    | 22:DA:201:C:C6     | 3.09                     | 0.40              |
| 22:DA:2066:C:O2'  | 22:DA:2067:G:H5'   | 2.21                     | 0.40              |
| 22:DA:2115:G:C4   | 22:DA:2117:A:C8    | 3.09                     | 0.40              |
| 22:DA:2345:G:C5   | 22:DA:2347:C:C5    | 3.09                     | 0.40              |
| 22:DA:2436:G:C2   | 22:DA:2437:G:C8    | 3.09                     | 0.40              |
| 22:DA:2526:G:O2'  | 52:D4:34:LYS:HE2   | 2.22                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:DA:1953:A:C2    | 22:DA:2550:G:O4'   | 2.74                     | 0.40              |
| 22:DA:2619:C:OP1   | 25:DD:157:LYS:HE2  | 2.21                     | 0.40              |
| 22:DA:2838:G:C6    | 22:DA:2839:G:C6    | 3.10                     | 0.40              |
| 22:DA:2881:U:H2'   | 22:DA:2882:A:C8    | 2.57                     | 0.40              |
| 22:DA:432:A:H2'    | 22:DA:433:C:C6     | 2.56                     | 0.40              |
| 22:DA:825:A:H4'    | 22:DA:2428:G:C5    | 2.56                     | 0.40              |
| 22:DA:600:G:C1'    | 26:DE:100:MET:HG2  | 2.51                     | 0.40              |
| 26:DE:108:ILE:HD13 | 26:DE:181:ILE:HG13 | 2.03                     | 0.40              |
| 29:DH:96:THR:O     | 29:DH:98:ASP:N     | 2.54                     | 0.40              |
| 30:DI:53:LEU:CG    | 30:DI:82:LYS:HE2   | 2.51                     | 0.40              |
| 31:DJ:38:GLY:O     | 31:DJ:40:HIS:N     | 2.54                     | 0.40              |
| 33:DL:29:LYS:CG    | 33:DL:29:LYS:O     | 2.68                     | 0.40              |
| 35:DN:20:MET:HG3   | 35:DN:21:PHE:N     | 2.36                     | 0.40              |
| 39:DR:85:LYS:HG2   | 39:DR:86:GLN:N     | 2.36                     | 0.40              |
| 41:DT:45:ALA:HA    | 41:DT:49:LYS:HE3   | 2.02                     | 0.40              |
| 41:DT:91:GLN:HG2   | 41:DT:91:GLN:O     | 2.20                     | 0.40              |
| 47:DZ:24:LEU:HD11  | 47:DZ:54:MET:CE    | 2.50                     | 0.40              |
| 1:AA:1072:G:H2'    | 1:AA:1073:U:C6     | 2.56                     | 0.40              |
| 1:AA:1133:G:C6     | 1:AA:1142:G:C6     | 3.09                     | 0.40              |
| 1:AA:1134:G:H2'    | 1:AA:1135:U:O4'    | 2.21                     | 0.40              |
| 1:AA:1126:U:O4'    | 1:AA:1281:C:C2     | 2.73                     | 0.40              |
| 1:AA:1301:U:C5     | 1:AA:1303:C:C4     | 3.09                     | 0.40              |
| 1:AA:935:A:O2'     | 1:AA:1383:C:O2     | 2.38                     | 0.40              |
| 1:AA:193:C:H2'     | 1:AA:194:C:H6      | 1.86                     | 0.40              |
| 1:AA:204:G:N2      | 1:AA:465:A:C8      | 2.89                     | 0.40              |
| 1:AA:273:U:C2'     | 1:AA:274:A:H5'     | 2.51                     | 0.40              |
| 1:AA:389:A:C6      | 1:AA:390:U:H1'     | 2.56                     | 0.40              |
| 1:AA:722:G:H2'     | 1:AA:723:U:OP2     | 2.21                     | 0.40              |
| 1:AA:666:G:C2      | 1:AA:741:G:C4      | 3.09                     | 0.40              |
| 1:AA:849:G:N1      | 1:AA:850:U:C2      | 2.90                     | 0.40              |
| 3:AC:167:TRP:HE3   | 3:AC:167:TRP:C     | 2.25                     | 0.40              |
| 13:AM:11:ASP:CG    | 13:AM:45:ILE:CG1   | 2.90                     | 0.40              |
| 14:AN:66:GLN:HG3   | 14:AN:79:LEU:HD21  | 2.03                     | 0.40              |
| 15:AO:82:ILE:HG22  | 15:AO:87:LEU:HD21  | 2.04                     | 0.40              |
| 16:AP:36:VAL:CG2   | 16:AP:57:ILE:HG13  | 2.51                     | 0.40              |
| 16:AP:77:GLU:C     | 16:AP:79:ASN:N     | 2.75                     | 0.40              |
| 17:AQ:13:VAL:HG12  | 17:AQ:22:VAL:O     | 2.21                     | 0.40              |
| 17:AQ:81:LYS:N     | 17:AQ:81:LYS:CD    | 2.85                     | 0.40              |
| 52:B4:36:ARG:HG2   | 52:B4:37:GLN:H     | 1.86                     | 0.40              |
| 22:BA:752:A:C2     | 22:BA:1781:U:N1    | 2.89                     | 0.40              |
| 22:BA:1842:G:H5''  | 22:BA:1843:C:OP2   | 2.21                     | 0.40              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 22:BA:2298:A:C2    | 22:BA:2321:U:C5    | 3.09                     | 0.40              |
| 22:BA:2031:A:C6    | 22:BA:2498:C:H1'   | 2.55                     | 0.40              |
| 22:BA:2564:A:OP1   | 22:BA:2648:G:H4'   | 2.21                     | 0.40              |
| 22:BA:272:A:H2'    | 22:BA:273:G:C8     | 2.56                     | 0.40              |
| 22:BA:2756:U:C1'   | 22:BA:2757:A:H5''  | 2.51                     | 0.40              |
| 22:BA:744:U:C4     | 22:BA:745:G:C5     | 3.09                     | 0.40              |
| 22:BA:995:C:O2     | 31:BJ:3:THR:OG1    | 2.32                     | 0.40              |
| 22:BA:1248:G:C5    | 26:BE:46:GLN:NE2   | 2.89                     | 0.40              |
| 27:BF:4:LEU:HD22   | 27:BF:173:PHE:CE2  | 2.56                     | 0.40              |
| 28:BG:25:THR:HG23  | 28:BG:34:THR:OG1   | 2.22                     | 0.40              |
| 28:BG:52:PHE:N     | 28:BG:52:PHE:CD2   | 2.90                     | 0.40              |
| 32:BK:66:LYS:HA    | 32:BK:79:PHE:O     | 2.21                     | 0.40              |
| 33:BL:120:VAL:HG22 | 33:BL:121:THR:N    | 2.36                     | 0.40              |
| 33:BL:38:GLN:O     | 33:BL:44:GLY:HA3   | 2.21                     | 0.40              |
| 35:BN:55:ALA:HB1   | 35:BN:80:PHE:N     | 2.36                     | 0.40              |
| 42:BU:8:ASP:OD2    | 42:BU:24:LYS:HD3   | 2.21                     | 0.40              |
| 44:BW:75:LYS:O     | 44:BW:76:ASN:HB2   | 2.21                     | 0.40              |
| 1:CA:1057:G:C5     | 1:CA:1204:A:C2     | 3.09                     | 0.40              |
| 1:CA:1129:C:C5     | 1:CA:1139:G:C8     | 3.09                     | 0.40              |
| 1:CA:116:A:H2'     | 1:CA:117:G:O5'     | 2.21                     | 0.40              |
| 1:CA:1386:G:O2'    | 1:CA:1387:G:H5'    | 2.21                     | 0.40              |
| 1:CA:53:A:H2'      | 1:CA:54:C:O4'      | 2.21                     | 0.40              |
| 1:CA:582:C:O2'     | 1:CA:583:A:H5'     | 2.21                     | 0.40              |
| 1:CA:583:A:C8      | 1:CA:584:G:C8      | 3.10                     | 0.40              |
| 1:CA:678:U:N3      | 1:CA:713:G:N2      | 2.70                     | 0.40              |
| 1:CA:890:G:H22     | 1:CA:906:A:H2'     | 1.85                     | 0.40              |
| 3:CC:130:PHE:CZ    | 3:CC:131:ARG:HD3   | 2.55                     | 0.40              |
| 7:CG:57:SER:HB3    | 7:CG:60:GLU:HB2    | 2.03                     | 0.40              |
| 9:CI:101:ALA:HB1   | 9:CI:103:PHE:CE1   | 2.56                     | 0.40              |
| 15:CO:16:GLY:O     | 15:CO:18:ASP:N     | 2.54                     | 0.40              |
| 17:CQ:44:LEU:O     | 17:CQ:46:VAL:HG23  | 2.21                     | 0.40              |
| 21:CU:36:GLU:HA    | 21:CU:36:GLU:OE1   | 2.20                     | 0.40              |
| 22:DA:1028:A:N6    | 22:DA:1125:G:H2'   | 2.36                     | 0.40              |
| 22:DA:1198:U:H2'   | 22:DA:1199:U:C6    | 2.56                     | 0.40              |
| 22:DA:144:A:N1     | 22:DA:145:C:C2     | 2.88                     | 0.40              |
| 22:DA:1999:C:H5''  | 22:DA:2723:C:O2'   | 2.22                     | 0.40              |
| 22:DA:2033:A:H4'   | 22:DA:2034:U:OP1   | 2.21                     | 0.40              |
| 22:DA:2050:C:C4    | 22:DA:2051:A:C6    | 3.09                     | 0.40              |
| 22:DA:2744:G:C6    | 22:DA:2761:A:C6    | 3.10                     | 0.40              |
| 55:DA:3001:DOL:O15 | 55:DA:3001:DOL:C21 | 2.62                     | 0.40              |
| 22:DA:445:C:H2'    | 22:DA:446:G:C8     | 2.56                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:DA:491:G:C2    | 22:DA:492:A:C4    | 3.09                     | 0.40              |
| 22:DA:681:G:N3    | 22:DA:682:G:C8    | 2.89                     | 0.40              |
| 23:DB:96:G:C2'    | 23:DB:97:C:H5'    | 2.51                     | 0.40              |
| 25:DD:140:HIS:CD2 | 25:DD:140:HIS:N   | 2.88                     | 0.40              |
| 26:DE:115:GLN:O   | 26:DE:117:ARG:HG3 | 2.22                     | 0.40              |
| 32:DK:35:VAL:HG22 | 32:DK:69:VAL:HG12 | 2.02                     | 0.40              |
| 33:DL:29:LYS:O    | 33:DL:29:LYS:HG2  | 2.22                     | 0.40              |
| 42:DU:82:ARG:O    | 42:DU:97:LYS:CB   | 2.70                     | 0.40              |
| 22:DA:380:G:O3'   | 45:DX:16:ASN:HB2  | 2.21                     | 0.40              |
| 46:DY:55:THR:O    | 46:DY:58:ASN:CB   | 2.70                     | 0.40              |
| 1:AA:1209:C:O2'   | 1:AA:1210:C:H5'   | 2.21                     | 0.40              |
| 1:AA:1319:A:C5    | 1:AA:1323:G:C4    | 3.10                     | 0.40              |
| 1:AA:1419:G:C4    | 1:AA:1420:U:C5    | 3.09                     | 0.40              |
| 1:AA:270:A:C5     | 1:AA:271:C:C4     | 3.09                     | 0.40              |
| 1:AA:397:A:C5     | 1:AA:548:G:N7     | 2.90                     | 0.40              |
| 1:AA:600:A:C2     | 1:AA:601:G:C4     | 3.09                     | 0.40              |
| 1:AA:945:G:H2'    | 1:AA:945:G:N3     | 2.37                     | 0.40              |
| 1:AA:957:U:H1'    | 1:AA:960:U:C4     | 2.56                     | 0.40              |
| 1:AA:982:U:H4'    | 1:AA:983:A:O5'    | 2.22                     | 0.40              |
| 2:AB:77:SER:O     | 2:AB:93:ASN:HB2   | 2.21                     | 0.40              |
| 4:AD:147:GLU:O    | 4:AD:150:LYS:HB2  | 2.21                     | 0.40              |
| 7:AG:122:ASN:O    | 7:AG:126:ASP:OD1  | 2.39                     | 0.40              |
| 8:AH:64:LYS:HB3   | 8:AH:64:LYS:HE2   | 1.94                     | 0.40              |
| 9:AI:28:ILE:HG13  | 9:AI:63:LEU:HD21  | 2.04                     | 0.40              |
| 10:AJ:32:THR:HG21 | 10:AJ:86:ALA:CB   | 2.51                     | 0.40              |
| 10:AJ:52:LEU:HD23 | 10:AJ:62:ARG:CG   | 2.50                     | 0.40              |
| 10:AJ:52:LEU:HD22 | 10:AJ:62:ARG:HG3  | 2.02                     | 0.40              |
| 14:AN:51:LEU:HB3  | 14:AN:52:PRO:HD2  | 2.03                     | 0.40              |
| 1:AA:451:A:H5''   | 16:AP:70:ARG:NH2  | 2.37                     | 0.40              |
| 17:AQ:49:GLU:O    | 17:AQ:51:ASN:N    | 2.54                     | 0.40              |
| 22:BA:1036:G:C5   | 22:BA:1120:G:C6   | 3.10                     | 0.40              |
| 22:BA:1178:C:O3'  | 22:BA:1179:G:C8   | 2.74                     | 0.40              |
| 22:BA:1301:A:C2   | 22:BA:1303:G:C6   | 3.10                     | 0.40              |
| 22:BA:1583:A:O2'  | 22:BA:1584:U:P    | 2.80                     | 0.40              |
| 22:BA:1840:G:C2'  | 22:BA:1841:U:H5'  | 2.52                     | 0.40              |
| 22:BA:1851:U:C2'  | 22:BA:1852:U:H5'  | 2.51                     | 0.40              |
| 22:BA:1920:C:O2   | 22:BA:1920:C:H2'  | 2.21                     | 0.40              |
| 22:BA:2297:A:C2   | 22:BA:2321:U:C5   | 3.09                     | 0.40              |
| 22:BA:2432:A:H2'  | 22:BA:2433:A:O4'  | 2.21                     | 0.40              |
| 22:BA:2512:C:H4'  | 25:BD:127:PHE:CE1 | 2.57                     | 0.40              |
| 22:BA:2627:G:N2   | 22:BA:2777:G:OP2  | 2.54                     | 0.40              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 22:BA:2900:A:H2'   | 22:BA:2901:C:O4'  | 2.22                     | 0.40              |
| 22:BA:64:A:C6      | 22:BA:65:U:C4     | 3.09                     | 0.40              |
| 22:BA:976:G:C2     | 22:BA:977:G:C8    | 3.09                     | 0.40              |
| 23:BB:111:U:H2'    | 23:BB:111:U:O2    | 2.21                     | 0.40              |
| 24:BC:172:VAL:HG23 | 24:BC:174:LEU:CD1 | 2.51                     | 0.40              |
| 22:BA:1205:A:C6    | 26:BE:165:HIS:HB2 | 2.57                     | 0.40              |
| 26:BE:97:ASN:O     | 26:BE:98:LYS:C    | 2.59                     | 0.40              |
| 27:BF:91:LEU:HB3   | 27:BF:96:MET:HA   | 2.03                     | 0.40              |
| 29:BH:120:GLY:HA2  | 29:BH:122:LEU:HA  | 2.04                     | 0.40              |
| 22:BA:1665:A:O2'   | 32:BK:1:MET:HB3   | 2.21                     | 0.40              |
| 35:BN:55:ALA:HB1   | 35:BN:80:PHE:H    | 1.87                     | 0.40              |
| 39:BR:49:ILE:HB    | 39:BR:52:PRO:CA   | 2.52                     | 0.40              |
| 1:CA:1179:A:C2'    | 1:CA:1180:A:H5'   | 2.52                     | 0.40              |
| 1:CA:1292:G:C2     | 1:CA:1293:C:C2    | 3.09                     | 0.40              |
| 1:CA:1352:C:C2     | 1:CA:1371:G:N1    | 2.89                     | 0.40              |
| 1:CA:861:G:N7      | 1:CA:862:C:C5     | 2.90                     | 0.40              |
| 1:CA:88:U:C5       | 1:CA:89:U:C5      | 3.09                     | 0.40              |
| 2:CB:56:GLU:OE2    | 2:CB:56:GLU:HA    | 2.22                     | 0.40              |
| 3:CC:117:ALA:HB1   | 3:CC:187:SER:CB   | 2.51                     | 0.40              |
| 3:CC:184:TYR:CD1   | 3:CC:201:TRP:NE1  | 2.89                     | 0.40              |
| 4:CD:106:GLY:O     | 4:CD:158:ALA:HB1  | 2.21                     | 0.40              |
| 6:CF:38:ARG:CG     | 6:CF:63:ASN:HB2   | 2.51                     | 0.40              |
| 9:CI:91:ASP:OD2    | 9:CI:91:ASP:C     | 2.59                     | 0.40              |
| 22:DA:684:G:OP1    | 50:D2:16:HIS:CE1  | 2.74                     | 0.40              |
| 22:DA:1187:G:H5''  | 39:DR:83:TYR:CZ   | 2.55                     | 0.40              |
| 22:DA:1316:U:H2'   | 22:DA:1317:G:C8   | 2.57                     | 0.40              |
| 22:DA:1340:U:O2    | 22:DA:1340:U:H2'  | 2.20                     | 0.40              |
| 22:DA:1651:G:C6    | 22:DA:1652:A:C5   | 3.09                     | 0.40              |
| 22:DA:201:C:H2'    | 22:DA:202:U:O5'   | 2.22                     | 0.40              |
| 22:DA:528:A:C2     | 22:DA:2043:C:C5'  | 3.05                     | 0.40              |
| 22:DA:2043:C:O2    | 22:DA:2044:C:C5   | 2.75                     | 0.40              |
| 22:DA:2756:U:C4    | 22:DA:2759:G:O6   | 2.75                     | 0.40              |
| 22:DA:590:A:H2'    | 22:DA:591:U:C6    | 2.56                     | 0.40              |
| 22:DA:922:C:H2'    | 22:DA:923:G:C8    | 2.57                     | 0.40              |
| 26:DE:8:ALA:CB     | 26:DE:122:GLU:CG  | 2.99                     | 0.40              |
| 31:DJ:35:ARG:CG    | 31:DJ:40:HIS:CD2  | 3.04                     | 0.40              |
| 33:DL:100:ILE:CG1  | 33:DL:100:ILE:O   | 2.69                     | 0.40              |
| 33:DL:29:LYS:O     | 33:DL:30:THR:OG1  | 2.25                     | 0.40              |
| 33:DL:29:LYS:O     | 33:DL:30:THR:HG23 | 2.22                     | 0.40              |
| 33:DL:68:SER:O     | 33:DL:69:ARG:HG3  | 2.21                     | 0.40              |
| 37:DP:51:ARG:CG    | 37:DP:51:ARG:O    | 2.69                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 40:DS:33:LEU:HD21 | 40:DS:52:GLU:CG   | 2.51                     | 0.40              |
| 1:AA:1030:U:H5'   | 1:AA:1031:C:OP1   | 2.22                     | 0.40              |
| 1:AA:1239:A:OP1   | 1:AA:1239:A:H4'   | 2.22                     | 0.40              |
| 1:AA:1316:G:N2    | 1:AA:1318:A:H3'   | 2.37                     | 0.40              |
| 1:AA:1376:U:H2'   | 1:AA:1377:A:C8    | 2.56                     | 0.40              |
| 1:AA:1383:C:H2'   | 1:AA:1384:C:C6    | 2.56                     | 0.40              |
| 1:AA:139:A:C2'    | 1:AA:140:U:H5'    | 2.51                     | 0.40              |
| 1:AA:201:G:H2'    | 1:AA:202:G:O4'    | 2.21                     | 0.40              |
| 1:AA:279:A:N3     | 1:AA:281:G:N2     | 2.69                     | 0.40              |
| 1:AA:324:G:N2     | 1:AA:326:G:H3'    | 2.36                     | 0.40              |
| 1:AA:557:G:C6     | 1:AA:558:G:N1     | 2.89                     | 0.40              |
| 1:AA:57:G:C6      | 1:AA:58:C:C4      | 3.09                     | 0.40              |
| 1:AA:606:G:H1'    | 1:AA:633:G:C2     | 2.56                     | 0.40              |
| 1:AA:69:G:C3'     | 1:AA:70:U:H6      | 2.34                     | 0.40              |
| 2:AB:49:MET:C     | 2:AB:51:ASN:O     | 2.60                     | 0.40              |
| 4:AD:29:ASP:O     | 4:AD:31:LYS:CE    | 2.70                     | 0.40              |
| 6:AF:72:ASP:O     | 6:AF:75:GLU:N     | 2.54                     | 0.40              |
| 8:AH:25:VAL:HG13  | 8:AH:25:VAL:O     | 2.21                     | 0.40              |
| 8:AH:43:GLU:HG3   | 8:AH:112:THR:HG21 | 2.03                     | 0.40              |
| 9:AI:51:PRO:HD3   | 9:AI:80:ARG:HG2   | 2.03                     | 0.40              |
| 1:AA:1125:U:O4'   | 10:AJ:73:LEU:CD1  | 2.70                     | 0.40              |
| 11:AK:38:GLN:O    | 11:AK:38:GLN:HG2  | 2.21                     | 0.40              |
| 12:AL:7:LEU:HD12  | 17:AQ:34:TYR:CE2  | 2.56                     | 0.40              |
| 1:AA:1302:C:C4    | 13:AM:17:ILE:HD13 | 2.56                     | 0.40              |
| 16:AP:20:VAL:CG2  | 16:AP:34:GLU:O    | 2.69                     | 0.40              |
| 21:AU:17:ARG:NH1  | 21:AU:20:LYS:HG3  | 2.36                     | 0.40              |
| 22:BA:2021:C:P    | 48:B0:9:THR:HG21  | 2.61                     | 0.40              |
| 51:B3:45:ARG:N    | 51:B3:46:PRO:HD2  | 2.37                     | 0.40              |
| 22:BA:1100:C:H2'  | 22:BA:1101:U:C6   | 2.56                     | 0.40              |
| 22:BA:1109:C:N4   | 22:BA:1110:G:N1   | 2.70                     | 0.40              |
| 22:BA:115:C:O2'   | 22:BA:116:C:H5'   | 2.22                     | 0.40              |
| 22:BA:565:C:H4'   | 22:BA:1253:A:N6   | 2.37                     | 0.40              |
| 22:BA:149:A:C5    | 22:BA:150:U:C5    | 3.10                     | 0.40              |
| 22:BA:1588:G:C4   | 22:BA:1589:U:C5   | 3.10                     | 0.40              |
| 22:BA:2010:G:H2'  | 22:BA:2011:U:O4'  | 2.21                     | 0.40              |
| 22:BA:2127:G:O2'  | 22:BA:2128:G:O4'  | 2.39                     | 0.40              |
| 22:BA:2232:C:C4   | 22:BA:2233:U:C5   | 3.10                     | 0.40              |
| 22:BA:2619:C:O2'  | 22:BA:2620:C:H5'  | 2.21                     | 0.40              |
| 22:BA:2741:A:H2'  | 22:BA:2742:G:O4'  | 2.21                     | 0.40              |
| 22:BA:319:G:C5    | 22:BA:333:G:N2    | 2.90                     | 0.40              |
| 22:BA:613:A:C8    | 22:BA:616:A:H2    | 2.38                     | 0.40              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 22:BA:634:C:H2'  | 22:BA:635:C:C6    | 2.57                     | 0.40              |
| 22:BA:735:A:N7   | 22:BA:761:A:H2    | 2.20                     | 0.40              |
| 23:BB:109:A:C6   | 23:BB:110:C:N3    | 2.90                     | 0.40              |
| 23:BB:30:C:O2'   | 23:BB:57:A:N1     | 2.45                     | 0.40              |
| 22:BA:2052:A:O4' | 25:BD:147:GLY:HA3 | 2.22                     | 0.40              |
| 26:BE:119:ILE:O  | 26:BE:187:VAL:HA  | 2.21                     | 0.40              |
| 36:BO:110:ALA:O  | 36:BO:115:LEU:HB3 | 2.20                     | 0.40              |
| 36:BO:12:THR:O   | 36:BO:12:THR:CG2  | 2.69                     | 0.40              |
| 36:BO:88:LYS:CG  | 36:BO:89:ASP:N    | 2.85                     | 0.40              |
| 37:BP:6:LYS:O    | 37:BP:7:GLN:C     | 2.59                     | 0.40              |
| 38:BQ:18:LEU:HA  | 38:BQ:18:LEU:HD13 | 1.99                     | 0.40              |
| 45:BX:45:ARG:HG2 | 45:BX:46:PHE:N    | 2.37                     | 0.40              |
| 46:BY:14:LEU:HG  | 46:BY:57:LEU:HD11 | 2.02                     | 0.40              |
| 47:BZ:5:ILE:HG23 | 47:BZ:40:ASP:HB2  | 2.04                     | 0.40              |
| 1:CA:1007:U:C3'  | 1:CA:1008:U:H5'   | 2.52                     | 0.40              |
| 1:CA:1070:U:H2'  | 1:CA:1071:C:C6    | 2.57                     | 0.40              |
| 1:CA:1434:A:N6   | 1:CA:1435:G:C6    | 2.89                     | 0.40              |
| 1:CA:1536:C:H2'  | 1:CA:1537:U:C6    | 2.56                     | 0.40              |
| 1:CA:1540:U:H4'  | 21:CU:18:ARG:HG2  | 2.02                     | 0.40              |
| 1:CA:223:A:C6    | 1:CA:224:U:C4     | 3.09                     | 0.40              |
| 1:CA:420:U:C2'   | 1:CA:421:U:H5''   | 2.51                     | 0.40              |
| 1:CA:496:A:N3    | 1:CA:497:G:N7     | 2.69                     | 0.40              |
| 1:CA:505:G:N3    | 1:CA:505:G:H2'    | 2.36                     | 0.40              |
| 1:CA:563:A:N7    | 1:CA:567:G:H1'    | 2.36                     | 0.40              |
| 1:CA:844:G:C8    | 1:CA:844:G:OP2    | 2.74                     | 0.40              |
| 1:CA:91:U:C4     | 1:CA:92:U:C5      | 3.10                     | 0.40              |
| 4:CD:195:ILE:O   | 4:CD:195:ILE:CG1  | 2.69                     | 0.40              |
| 4:CD:24:GLY:O    | 4:CD:161:LEU:CD1  | 2.70                     | 0.40              |
| 4:CD:91:LEU:HD12 | 4:CD:188:ARG:NE   | 2.37                     | 0.40              |
| 6:CF:71:ILE:N    | 6:CF:71:ILE:CD1   | 2.85                     | 0.40              |
| 7:CG:148:ASN:C   | 7:CG:150:ALA:N    | 2.75                     | 0.40              |
| 9:CI:31:ASN:HA   | 9:CI:66:THR:HG22  | 2.03                     | 0.40              |
| 9:CI:61:LEU:N    | 9:CI:61:LEU:CD2   | 2.85                     | 0.40              |
| 9:CI:76:ALA:HA   | 9:CI:79:ILE:HD12  | 2.03                     | 0.40              |
| 12:CL:79:VAL:O   | 12:CL:103:ASP:HB2 | 2.21                     | 0.40              |
| 13:CM:13:LYS:O   | 13:CM:14:HIS:CG   | 2.72                     | 0.40              |
| 13:CM:24:GLY:HA3 | 13:CM:65:VAL:HG12 | 2.04                     | 0.40              |
| 15:CO:57:LEU:O   | 15:CO:61:SER:N    | 2.46                     | 0.40              |
| 18:CR:49:ALA:O   | 18:CR:50:LYS:C    | 2.58                     | 0.40              |
| 22:DA:1263:U:H4' | 48:D0:7:LYS:HE3   | 2.04                     | 0.40              |
| 22:DA:1275:A:H4' | 22:DA:1276:A:OP1  | 2.19                     | 0.40              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 22:DA:1358:G:N2   | 22:DA:1374:G:C6   | 2.90                     | 0.40              |
| 22:DA:1359:A:C5   | 22:DA:1360:G:C8   | 3.09                     | 0.40              |
| 22:DA:1409:U:H2'  | 22:DA:1410:G:C8   | 2.56                     | 0.40              |
| 22:DA:1437:C:C4   | 22:DA:1438:U:O4   | 2.75                     | 0.40              |
| 22:DA:1737:G:C6   | 22:DA:1738:G:C6   | 3.10                     | 0.40              |
| 22:DA:190:A:N6    | 22:DA:191:A:N1    | 2.70                     | 0.40              |
| 22:DA:1924:C:H2'  | 22:DA:1925:C:O4'  | 2.21                     | 0.40              |
| 22:DA:211:C:H2'   | 22:DA:212:G:O4'   | 2.21                     | 0.40              |
| 22:DA:2234:G:C6   | 22:DA:2235:G:C8   | 3.10                     | 0.40              |
| 22:DA:2677:G:H2'  | 22:DA:2678:C:C6   | 2.56                     | 0.40              |
| 22:DA:299:A:C2    | 22:DA:319:G:N3    | 2.89                     | 0.40              |
| 22:DA:422:A:N1    | 22:DA:423:A:C4    | 2.89                     | 0.40              |
| 22:DA:476:G:H4'   | 22:DA:502:A:N1    | 2.36                     | 0.40              |
| 22:DA:540:C:C2    | 22:DA:541:A:C8    | 3.10                     | 0.40              |
| 22:DA:563:A:C2    | 22:DA:2018:G:H1'  | 2.56                     | 0.40              |
| 22:DA:756:A:H2'   | 22:DA:757:G:O4'   | 2.21                     | 0.40              |
| 22:DA:690:G:O2'   | 22:DA:780:G:OP1   | 2.29                     | 0.40              |
| 22:DA:7:G:H4'     | 31:DJ:15:TRP:HH2  | 1.87                     | 0.40              |
| 23:DB:44:G:N2     | 23:DB:48:U:C2     | 2.89                     | 0.40              |
| 25:DD:62:LYS:N    | 25:DD:63:PRO:CD   | 2.84                     | 0.40              |
| 26:DE:18:THR:O    | 26:DE:110:SER:OG  | 2.40                     | 0.40              |
| 22:DA:320:A:H2'   | 26:DE:131:THR:CG2 | 2.52                     | 0.40              |
| 26:DE:52:VAL:HB   | 26:DE:74:LYS:HD3  | 2.03                     | 0.40              |
| 31:DJ:17:VAL:HG23 | 31:DJ:137:PRO:HB2 | 2.03                     | 0.40              |
| 32:DK:31:ARG:HB2  | 32:DK:32:TYR:CD2  | 2.56                     | 0.40              |
| 37:DP:28:VAL:HG21 | 37:DP:74:PHE:CE2  | 2.56                     | 0.40              |
| 39:DR:51:VAL:O    | 39:DR:52:PRO:C    | 2.58                     | 0.40              |
| 41:DT:2:ILE:HG12  | 41:DT:7:LEU:CD1   | 2.52                     | 0.40              |
| 41:DT:2:ILE:HG12  | 41:DT:7:LEU:HD12  | 2.02                     | 0.40              |
| 41:DT:93:LEU:HD22 | 41:DT:93:LEU:N    | 2.36                     | 0.40              |
| 42:DU:38:GLY:HA2  | 42:DU:41:LEU:HD21 | 2.01                     | 0.40              |
| 45:DX:58:VAL:CG1  | 45:DX:59:ILE:N    | 2.85                     | 0.40              |
| 22:DA:61:C:OP1    | 46:DY:44:LYS:HD3  | 2.21                     | 0.40              |

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1         | Atom-2                 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|------------------------|--------------------------|-------------------|
| 1:AA:357:G:O2' | 29:DH:91:PHE:O[4_455]  | 2.12                     | 0.08              |
| 1:AA:368:U:OP1 | 29:DH:93:SER:OG[4_455] | 2.16                     | 0.04              |
| 1:AA:359:G:OP1 | 29:DH:89:LYS:NZ[4_455] | 2.17                     | 0.03              |

## 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 X-ray entries followed by that with respect to entries of similar resolution.

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 |   |
|-----|-------|---------------|-----------|----------|----------|-------------|---|
| 2   | AB    | 216/218 (99%) | 132 (61%) | 40 (18%) | 44 (20%) | 0           | 0 |
| 2   | CB    | 216/218 (99%) | 142 (66%) | 48 (22%) | 26 (12%) | 0           | 1 |
| 3   | AC    | 204/206 (99%) | 149 (73%) | 31 (15%) | 24 (12%) | 0           | 1 |
| 3   | CC    | 204/206 (99%) | 154 (76%) | 39 (19%) | 11 (5%)  | 2           | 6 |
| 4   | AD    | 203/205 (99%) | 133 (66%) | 45 (22%) | 25 (12%) | 0           | 1 |
| 4   | CD    | 203/205 (99%) | 147 (72%) | 33 (16%) | 23 (11%) | 0           | 1 |
| 5   | AE    | 148/150 (99%) | 102 (69%) | 23 (16%) | 23 (16%) | 0           | 0 |
| 5   | CE    | 148/150 (99%) | 98 (66%)  | 34 (23%) | 16 (11%) | 0           | 1 |
| 6   | AF    | 98/100 (98%)  | 67 (68%)  | 22 (22%) | 9 (9%)   | 1           | 1 |
| 6   | CF    | 98/100 (98%)  | 66 (67%)  | 18 (18%) | 14 (14%) | 0           | 0 |
| 7   | AG    | 149/151 (99%) | 110 (74%) | 26 (17%) | 13 (9%)  | 1           | 2 |
| 7   | CG    | 149/151 (99%) | 120 (80%) | 20 (13%) | 9 (6%)   | 1           | 4 |
| 8   | AH    | 127/129 (98%) | 87 (68%)  | 31 (24%) | 9 (7%)   | 1           | 3 |
| 8   | CH    | 127/129 (98%) | 102 (80%) | 17 (13%) | 8 (6%)   | 1           | 4 |
| 9   | AI    | 125/127 (98%) | 88 (70%)  | 23 (18%) | 14 (11%) | 0           | 1 |
| 9   | CI    | 125/127 (98%) | 89 (71%)  | 21 (17%) | 15 (12%) | 0           | 1 |
| 10  | AJ    | 96/98 (98%)   | 62 (65%)  | 14 (15%) | 20 (21%) | 0           | 0 |
| 10  | CJ    | 96/98 (98%)   | 74 (77%)  | 10 (10%) | 12 (12%) | 0           | 0 |
| 11  | AK    | 115/117 (98%) | 81 (70%)  | 15 (13%) | 19 (16%) | 0           | 0 |
| 11  | CK    | 115/117 (98%) | 80 (70%)  | 26 (23%) | 9 (8%)   | 1           | 2 |
| 12  | AL    | 121/123 (98%) | 91 (75%)  | 20 (16%) | 10 (8%)  | 1           | 2 |
| 12  | CL    | 121/123 (98%) | 89 (74%)  | 20 (16%) | 12 (10%) | 0           | 1 |
| 13  | AM    | 112/114 (98%) | 80 (71%)  | 21 (19%) | 11 (10%) | 0           | 1 |
| 13  | CM    | 112/114 (98%) | 82 (73%)  | 17 (15%) | 13 (12%) | 0           | 1 |
| 14  | AN    | 92/100 (92%)  | 54 (59%)  | 29 (32%) | 9 (10%)  | 0           | 1 |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 14  | CN    | 92/100 (92%)  | 56 (61%)  | 22 (24%) | 14 (15%) | 0           | 0  |
| 15  | AO    | 86/88 (98%)   | 61 (71%)  | 19 (22%) | 6 (7%)   | 1           | 3  |
| 15  | CO    | 86/88 (98%)   | 66 (77%)  | 16 (19%) | 4 (5%)   | 2           | 8  |
| 16  | AP    | 80/82 (98%)   | 57 (71%)  | 11 (14%) | 12 (15%) | 0           | 0  |
| 16  | CP    | 80/82 (98%)   | 59 (74%)  | 16 (20%) | 5 (6%)   | 1           | 4  |
| 17  | AQ    | 78/80 (98%)   | 55 (70%)  | 15 (19%) | 8 (10%)  | 0           | 1  |
| 17  | CQ    | 78/80 (98%)   | 58 (74%)  | 11 (14%) | 9 (12%)  | 0           | 1  |
| 18  | AR    | 53/55 (96%)   | 41 (77%)  | 10 (19%) | 2 (4%)   | 3           | 13 |
| 18  | CR    | 53/55 (96%)   | 34 (64%)  | 16 (30%) | 3 (6%)   | 1           | 5  |
| 19  | AS    | 77/79 (98%)   | 55 (71%)  | 13 (17%) | 9 (12%)  | 0           | 1  |
| 19  | CS    | 77/79 (98%)   | 56 (73%)  | 12 (16%) | 9 (12%)  | 0           | 1  |
| 20  | AT    | 83/85 (98%)   | 57 (69%)  | 20 (24%) | 6 (7%)   | 1           | 3  |
| 20  | CT    | 83/85 (98%)   | 64 (77%)  | 10 (12%) | 9 (11%)  | 0           | 1  |
| 21  | AU    | 49/51 (96%)   | 28 (57%)  | 8 (16%)  | 13 (26%) | 0           | 0  |
| 21  | CU    | 49/51 (96%)   | 26 (53%)  | 10 (20%) | 13 (26%) | 0           | 0  |
| 24  | BC    | 269/271 (99%) | 219 (81%) | 38 (14%) | 12 (4%)  | 2           | 9  |
| 24  | DC    | 269/271 (99%) | 195 (72%) | 50 (19%) | 24 (9%)  | 1           | 1  |
| 25  | BD    | 207/209 (99%) | 178 (86%) | 22 (11%) | 7 (3%)   | 3           | 15 |
| 25  | DD    | 207/209 (99%) | 153 (74%) | 45 (22%) | 9 (4%)   | 2           | 10 |
| 26  | BE    | 199/201 (99%) | 162 (81%) | 34 (17%) | 3 (2%)   | 10          | 34 |
| 26  | DE    | 199/201 (99%) | 153 (77%) | 29 (15%) | 17 (8%)  | 1           | 2  |
| 27  | BF    | 175/177 (99%) | 139 (79%) | 28 (16%) | 8 (5%)   | 2           | 9  |
| 27  | DF    | 175/177 (99%) | 140 (80%) | 23 (13%) | 12 (7%)  | 1           | 3  |
| 28  | BG    | 174/176 (99%) | 147 (84%) | 18 (10%) | 9 (5%)   | 2           | 6  |
| 28  | DG    | 174/176 (99%) | 130 (75%) | 29 (17%) | 15 (9%)  | 1           | 2  |
| 29  | BH    | 147/149 (99%) | 89 (60%)  | 37 (25%) | 21 (14%) | 0           | 0  |
| 29  | DH    | 147/149 (99%) | 100 (68%) | 32 (22%) | 15 (10%) | 0           | 1  |
| 30  | BI    | 139/141 (99%) | 81 (58%)  | 34 (24%) | 24 (17%) | 0           | 0  |
| 30  | DI    | 139/141 (99%) | 81 (58%)  | 38 (27%) | 20 (14%) | 0           | 0  |
| 31  | BJ    | 140/142 (99%) | 130 (93%) | 7 (5%)   | 3 (2%)   | 7           | 26 |
| 31  | DJ    | 140/142 (99%) | 112 (80%) | 14 (10%) | 14 (10%) | 0           | 1  |

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| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |     |
|-----|-------|---------------|-----------|----------|----------|-------------|-----|
| 32  | BK    | 120/122 (98%) | 97 (81%)  | 16 (13%) | 7 (6%)   | 1           | 5   |
| 32  | DK    | 120/122 (98%) | 97 (81%)  | 13 (11%) | 10 (8%)  | 1           | 2   |
| 33  | BL    | 141/143 (99%) | 118 (84%) | 18 (13%) | 5 (4%)   | 3           | 14  |
| 33  | DL    | 141/143 (99%) | 101 (72%) | 25 (18%) | 15 (11%) | 0           | 1   |
| 34  | BM    | 134/136 (98%) | 118 (88%) | 14 (10%) | 2 (2%)   | 10          | 34  |
| 34  | DM    | 134/136 (98%) | 108 (81%) | 19 (14%) | 7 (5%)   | 2           | 6   |
| 35  | BN    | 118/120 (98%) | 99 (84%)  | 16 (14%) | 3 (2%)   | 5           | 21  |
| 35  | DN    | 118/120 (98%) | 92 (78%)  | 16 (14%) | 10 (8%)  | 1           | 2   |
| 36  | BO    | 114/116 (98%) | 94 (82%)  | 17 (15%) | 3 (3%)   | 5           | 20  |
| 36  | DO    | 114/116 (98%) | 84 (74%)  | 23 (20%) | 7 (6%)   | 1           | 4   |
| 37  | BP    | 112/114 (98%) | 96 (86%)  | 10 (9%)  | 6 (5%)   | 2           | 6   |
| 37  | DP    | 112/114 (98%) | 86 (77%)  | 19 (17%) | 7 (6%)   | 1           | 4   |
| 38  | BQ    | 115/117 (98%) | 109 (95%) | 4 (4%)   | 2 (2%)   | 9           | 31  |
| 38  | DQ    | 115/117 (98%) | 93 (81%)  | 20 (17%) | 2 (2%)   | 9           | 31  |
| 39  | BR    | 101/103 (98%) | 81 (80%)  | 10 (10%) | 10 (10%) | 0           | 1   |
| 39  | DR    | 101/103 (98%) | 73 (72%)  | 22 (22%) | 6 (6%)   | 1           | 5   |
| 40  | BS    | 108/110 (98%) | 92 (85%)  | 13 (12%) | 3 (3%)   | 5           | 19  |
| 40  | DS    | 108/110 (98%) | 83 (77%)  | 17 (16%) | 8 (7%)   | 1           | 2   |
| 41  | BT    | 91/93 (98%)   | 74 (81%)  | 8 (9%)   | 9 (10%)  | 0           | 1   |
| 41  | DT    | 91/93 (98%)   | 53 (58%)  | 26 (29%) | 12 (13%) | 0           | 0   |
| 42  | BU    | 100/102 (98%) | 77 (77%)  | 17 (17%) | 6 (6%)   | 1           | 4   |
| 42  | DU    | 100/102 (98%) | 69 (69%)  | 17 (17%) | 14 (14%) | 0           | 0   |
| 43  | BV    | 92/94 (98%)   | 84 (91%)  | 6 (6%)   | 2 (2%)   | 6           | 24  |
| 43  | DV    | 92/94 (98%)   | 77 (84%)  | 12 (13%) | 3 (3%)   | 4           | 15  |
| 44  | BW    | 74/76 (97%)   | 68 (92%)  | 6 (8%)   | 0        | 100         | 100 |
| 44  | DW    | 73/76 (96%)   | 60 (82%)  | 13 (18%) | 0        | 100         | 100 |
| 45  | BX    | 75/77 (97%)   | 66 (88%)  | 8 (11%)  | 1 (1%)   | 12          | 37  |
| 45  | DX    | 75/77 (97%)   | 57 (76%)  | 11 (15%) | 7 (9%)   | 0           | 1   |
| 46  | BY    | 61/63 (97%)   | 42 (69%)  | 11 (18%) | 8 (13%)  | 0           | 0   |
| 46  | DY    | 61/63 (97%)   | 46 (75%)  | 12 (20%) | 3 (5%)   | 2           | 8   |
| 47  | BZ    | 56/58 (97%)   | 51 (91%)  | 3 (5%)   | 2 (4%)   | 3           | 14  |

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| Mol | Chain | Analysed          | Favoured   | Allowed    | Outliers | Percentiles |    |
|-----|-------|-------------------|------------|------------|----------|-------------|----|
| 47  | DZ    | 56/58 (97%)       | 45 (80%)   | 7 (12%)    | 4 (7%)   | 1           | 3  |
| 48  | B0    | 54/56 (96%)       | 47 (87%)   | 4 (7%)     | 3 (6%)   | 2           | 5  |
| 48  | D0    | 54/56 (96%)       | 38 (70%)   | 12 (22%)   | 4 (7%)   | 1           | 2  |
| 49  | B1    | 48/50 (96%)       | 38 (79%)   | 7 (15%)    | 3 (6%)   | 1           | 4  |
| 49  | D1    | 48/50 (96%)       | 39 (81%)   | 4 (8%)     | 5 (10%)  | 0           | 1  |
| 50  | B2    | 44/46 (96%)       | 38 (86%)   | 4 (9%)     | 2 (4%)   | 2           | 9  |
| 50  | D2    | 44/46 (96%)       | 32 (73%)   | 8 (18%)    | 4 (9%)   | 1           | 1  |
| 51  | B3    | 62/64 (97%)       | 56 (90%)   | 5 (8%)     | 1 (2%)   | 9           | 32 |
| 51  | D3    | 62/64 (97%)       | 49 (79%)   | 11 (18%)   | 2 (3%)   | 4           | 16 |
| 52  | B4    | 36/38 (95%)       | 31 (86%)   | 4 (11%)    | 1 (3%)   | 5           | 19 |
| 52  | D4    | 36/38 (95%)       | 31 (86%)   | 3 (8%)     | 2 (6%)   | 2           | 5  |
| 53  | B5    | 183/228 (80%)     | 85 (46%)   | 59 (32%)   | 39 (21%) | 0           | 0  |
| All | All   | 11418/11672 (98%) | 8535 (75%) | 1900 (17%) | 983 (9%) | 1           | 2  |

All (983) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | AB    | 16  | PHE  |
| 2   | AB    | 22  | TYR  |
| 2   | AB    | 25  | PRO  |
| 2   | AB    | 34  | ALA  |
| 2   | AB    | 64  | LYS  |
| 2   | AB    | 73  | LYS  |
| 2   | AB    | 74  | ARG  |
| 2   | AB    | 75  | ALA  |
| 2   | AB    | 76  | ALA  |
| 2   | AB    | 88  | ASP  |
| 2   | AB    | 107 | VAL  |
| 2   | AB    | 120 | GLN  |
| 2   | AB    | 126 | PHE  |
| 2   | AB    | 134 | ALA  |
| 2   | AB    | 148 | LEU  |
| 2   | AB    | 152 | LYS  |
| 2   | AB    | 155 | GLY  |
| 2   | AB    | 194 | ASP  |
| 2   | AB    | 201 | PRO  |
| 3   | AC    | 12  | LEU  |
| 3   | AC    | 15  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | AC    | 17  | PRO  |
| 3   | AC    | 18  | TRP  |
| 3   | AC    | 26  | THR  |
| 3   | AC    | 61  | ALA  |
| 3   | AC    | 80  | LYS  |
| 3   | AC    | 140 | ASN  |
| 3   | AC    | 141 | ALA  |
| 3   | AC    | 146 | ALA  |
| 4   | AD    | 23  | SER  |
| 4   | AD    | 25  | VAL  |
| 4   | AD    | 29  | ASP  |
| 4   | AD    | 33  | LYS  |
| 4   | AD    | 35  | GLU  |
| 4   | AD    | 85  | ASN  |
| 4   | AD    | 121 | LYS  |
| 4   | AD    | 126 | ASN  |
| 4   | AD    | 153 | SER  |
| 4   | AD    | 168 | PRO  |
| 4   | AD    | 191 | LEU  |
| 4   | AD    | 192 | SER  |
| 5   | AE    | 26  | LYS  |
| 5   | AE    | 69  | ARG  |
| 5   | AE    | 70  | ASN  |
| 5   | AE    | 100 | SER  |
| 5   | AE    | 138 | ARG  |
| 5   | AE    | 158 | GLY  |
| 6   | AF    | 91  | ARG  |
| 6   | AF    | 92  | THR  |
| 6   | AF    | 99  | ALA  |
| 7   | AG    | 9   | GLN  |
| 7   | AG    | 14  | PRO  |
| 7   | AG    | 15  | ASP  |
| 7   | AG    | 56  | LYS  |
| 7   | AG    | 57  | SER  |
| 7   | AG    | 81  | GLY  |
| 7   | AG    | 100 | ALA  |
| 7   | AG    | 130 | ASN  |
| 9   | AI    | 41  | ARG  |
| 9   | AI    | 44  | ALA  |
| 9   | AI    | 58  | VAL  |
| 9   | AI    | 59  | GLU  |
| 10  | AJ    | 34  | ALA  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10  | AJ    | 35  | GLN  |
| 10  | AJ    | 57  | VAL  |
| 10  | AJ    | 74  | VAL  |
| 10  | AJ    | 93  | ALA  |
| 10  | AJ    | 101 | SER  |
| 11  | AK    | 27  | PHE  |
| 11  | AK    | 39  | GLY  |
| 11  | AK    | 41  | ALA  |
| 11  | AK    | 52  | PHE  |
| 11  | AK    | 56  | ARG  |
| 11  | AK    | 73  | ALA  |
| 11  | AK    | 103 | ALA  |
| 11  | AK    | 126 | LYS  |
| 12  | AL    | 24  | LEU  |
| 12  | AL    | 44  | LYS  |
| 12  | AL    | 89  | ASP  |
| 13  | AM    | 5   | ALA  |
| 13  | AM    | 12  | HIS  |
| 13  | AM    | 107 | ARG  |
| 13  | AM    | 114 | LYS  |
| 14  | AN    | 34  | VAL  |
| 14  | AN    | 42  | TRP  |
| 14  | AN    | 47  | LYS  |
| 14  | AN    | 52  | PRO  |
| 14  | AN    | 62  | ASN  |
| 15  | AO    | 17  | ARG  |
| 16  | AP    | 43  | ALA  |
| 16  | AP    | 46  | LYS  |
| 16  | AP    | 80  | LYS  |
| 17  | AQ    | 13  | VAL  |
| 17  | AQ    | 51  | ASN  |
| 17  | AQ    | 82  | ALA  |
| 19  | AS    | 6   | LYS  |
| 19  | AS    | 23  | VAL  |
| 19  | AS    | 64  | ASP  |
| 19  | AS    | 65  | GLU  |
| 20  | AT    | 4   | ILE  |
| 20  | AT    | 6   | SER  |
| 21  | AU    | 9   | ASN  |
| 21  | AU    | 12  | PHE  |
| 21  | AU    | 24  | GLU  |
| 21  | AU    | 35  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 21  | AU    | 36  | GLU  |
| 21  | AU    | 37  | PHE  |
| 21  | AU    | 40  | LYS  |
| 24  | BC    | 71  | LYS  |
| 24  | BC    | 122 | ALA  |
| 24  | BC    | 196 | GLY  |
| 24  | BC    | 253 | LYS  |
| 25  | BD    | 86  | GLU  |
| 25  | BD    | 152 | PRO  |
| 26  | BE    | 86  | ALA  |
| 27  | BF    | 3   | LYS  |
| 27  | BF    | 41  | GLY  |
| 27  | BF    | 175 | PHE  |
| 28  | BG    | 110 | SER  |
| 28  | BG    | 119 | ALA  |
| 28  | BG    | 175 | LYS  |
| 29  | BH    | 10  | ALA  |
| 29  | BH    | 34  | GLY  |
| 29  | BH    | 53  | GLU  |
| 29  | BH    | 87  | GLU  |
| 29  | BH    | 90  | LEU  |
| 29  | BH    | 118 | PRO  |
| 29  | BH    | 121 | VAL  |
| 29  | BH    | 140 | ALA  |
| 30  | BI    | 19  | ASN  |
| 30  | BI    | 45  | LYS  |
| 30  | BI    | 63  | ALA  |
| 30  | BI    | 83  | ALA  |
| 30  | BI    | 86  | ILE  |
| 30  | BI    | 113 | LYS  |
| 30  | BI    | 117 | MET  |
| 32  | BK    | 35  | VAL  |
| 32  | BK    | 108 | ARG  |
| 33  | BL    | 69  | ARG  |
| 33  | BL    | 94  | THR  |
| 34  | BM    | 69  | PRO  |
| 37  | BP    | 114 | LEU  |
| 38  | BQ    | 25  | TYR  |
| 39  | BR    | 29  | THR  |
| 39  | BR    | 31  | GLU  |
| 39  | BR    | 49  | ILE  |
| 39  | BR    | 51  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 39  | BR    | 53  | PHE  |
| 40  | BS    | 64  | ALA  |
| 41  | BT    | 2   | ILE  |
| 41  | BT    | 17  | SER  |
| 41  | BT    | 25  | GLU  |
| 41  | BT    | 89  | GLU  |
| 42  | BU    | 21  | LYS  |
| 42  | BU    | 52  | LEU  |
| 45  | BX    | 3   | ARG  |
| 46  | BY    | 22  | LEU  |
| 46  | BY    | 23  | ARG  |
| 46  | BY    | 36  | GLN  |
| 46  | BY    | 58  | ASN  |
| 46  | BY    | 62  | GLY  |
| 49  | B1    | 5   | ILE  |
| 49  | B1    | 17  | THR  |
| 50  | B2    | 44  | VAL  |
| 53  | B5    | 53  | ARG  |
| 53  | B5    | 60  | ARG  |
| 53  | B5    | 86  | GLU  |
| 53  | B5    | 126 | SER  |
| 53  | B5    | 134 | PRO  |
| 53  | B5    | 141 | PRO  |
| 53  | B5    | 167 | ASP  |
| 53  | B5    | 173 | HIS  |
| 53  | B5    | 175 | PRO  |
| 53  | B5    | 183 | PRO  |
| 53  | B5    | 184 | GLU  |
| 53  | B5    | 185 | LYS  |
| 53  | B5    | 203 | GLU  |
| 53  | B5    | 209 | PHE  |
| 53  | B5    | 214 | TYR  |
| 53  | B5    | 215 | VAL  |
| 53  | B5    | 216 | THR  |
| 53  | B5    | 221 | PRO  |
| 2   | CB    | 16  | PHE  |
| 2   | CB    | 35  | ARG  |
| 2   | CB    | 36  | ASN  |
| 2   | CB    | 74  | ARG  |
| 2   | CB    | 87  | CYS  |
| 2   | CB    | 88  | ASP  |
| 2   | CB    | 120 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | CB    | 126 | PHE  |
| 2   | CB    | 141 | LEU  |
| 2   | CB    | 168 | HIS  |
| 2   | CB    | 194 | ASP  |
| 2   | CB    | 207 | ILE  |
| 2   | CB    | 220 | THR  |
| 3   | CC    | 82  | GLU  |
| 3   | CC    | 127 | ARG  |
| 3   | CC    | 146 | ALA  |
| 4   | CD    | 28  | ILE  |
| 4   | CD    | 30  | THR  |
| 4   | CD    | 32  | CYS  |
| 4   | CD    | 33  | LYS  |
| 4   | CD    | 35  | GLU  |
| 4   | CD    | 42  | GLY  |
| 4   | CD    | 169 | THR  |
| 4   | CD    | 175 | ALA  |
| 5   | CE    | 100 | SER  |
| 5   | CE    | 101 | GLU  |
| 5   | CE    | 102 | GLY  |
| 5   | CE    | 103 | THR  |
| 5   | CE    | 123 | VAL  |
| 5   | CE    | 158 | GLY  |
| 6   | CF    | 33  | GLU  |
| 6   | CF    | 55  | HIS  |
| 6   | CF    | 56  | LYS  |
| 6   | CF    | 65  | GLU  |
| 6   | CF    | 92  | THR  |
| 6   | CF    | 98  | GLU  |
| 6   | CF    | 99  | ALA  |
| 7   | CG    | 3   | ARG  |
| 7   | CG    | 130 | ASN  |
| 7   | CG    | 146 | GLU  |
| 8   | CH    | 3   | MET  |
| 9   | CI    | 26  | GLY  |
| 9   | CI    | 41  | ARG  |
| 9   | CI    | 53  | GLU  |
| 9   | CI    | 91  | ASP  |
| 9   | CI    | 120 | LYS  |
| 10  | CJ    | 91  | ASP  |
| 11  | CK    | 52  | PHE  |
| 11  | CK    | 93  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11  | CK    | 127 | ARG  |
| 12  | CL    | 4   | VAL  |
| 12  | CL    | 44  | LYS  |
| 12  | CL    | 48  | ALA  |
| 12  | CL    | 58  | THR  |
| 12  | CL    | 89  | ASP  |
| 13  | CM    | 7   | ILE  |
| 13  | CM    | 41  | GLU  |
| 13  | CM    | 99  | GLY  |
| 14  | CN    | 22  | ALA  |
| 14  | CN    | 29  | ALA  |
| 14  | CN    | 32  | SER  |
| 14  | CN    | 52  | PRO  |
| 14  | CN    | 59  | ARG  |
| 14  | CN    | 81  | ARG  |
| 14  | CN    | 92  | GLU  |
| 15  | CO    | 14  | GLU  |
| 15  | CO    | 18  | ASP  |
| 17  | CQ    | 51  | ASN  |
| 17  | CQ    | 70  | THR  |
| 17  | CQ    | 76  | VAL  |
| 18  | CR    | 21  | ILE  |
| 18  | CR    | 25  | ASP  |
| 19  | CS    | 5   | LEU  |
| 19  | CS    | 32  | ARG  |
| 20  | CT    | 4   | ILE  |
| 20  | CT    | 6   | SER  |
| 20  | CT    | 68  | HIS  |
| 21  | CU    | 9   | ASN  |
| 21  | CU    | 12  | PHE  |
| 21  | CU    | 13  | ASP  |
| 21  | CU    | 24  | GLU  |
| 21  | CU    | 36  | GLU  |
| 21  | CU    | 37  | PHE  |
| 21  | CU    | 40  | LYS  |
| 21  | CU    | 52  | ALA  |
| 24  | DC    | 10  | SER  |
| 24  | DC    | 19  | VAL  |
| 24  | DC    | 29  | PRO  |
| 24  | DC    | 35  | GLU  |
| 24  | DC    | 58  | HIS  |
| 24  | DC    | 71  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 24  | DC    | 122 | ALA  |
| 24  | DC    | 238 | ARG  |
| 25  | DD    | 36  | GLN  |
| 25  | DD    | 57  | ALA  |
| 25  | DD    | 98  | VAL  |
| 25  | DD    | 105 | LYS  |
| 25  | DD    | 151 | THR  |
| 25  | DD    | 152 | PRO  |
| 27  | DF    | 122 | PHE  |
| 27  | DF    | 123 | ASP  |
| 27  | DF    | 175 | PHE  |
| 28  | DG    | 92  | VAL  |
| 28  | DG    | 119 | ALA  |
| 28  | DG    | 159 | GLY  |
| 29  | DH    | 3   | VAL  |
| 29  | DH    | 10  | ALA  |
| 29  | DH    | 33  | GLN  |
| 29  | DH    | 35  | LYS  |
| 29  | DH    | 41  | LYS  |
| 29  | DH    | 53  | GLU  |
| 29  | DH    | 54  | LEU  |
| 29  | DH    | 83  | LYS  |
| 29  | DH    | 109 | GLU  |
| 30  | DI    | 3   | LYS  |
| 30  | DI    | 7   | ALA  |
| 30  | DI    | 19  | ASN  |
| 30  | DI    | 93  | PRO  |
| 30  | DI    | 101 | ILE  |
| 30  | DI    | 102 | SER  |
| 30  | DI    | 115 | ALA  |
| 31  | DJ    | 6   | ALA  |
| 31  | DJ    | 11  | VAL  |
| 31  | DJ    | 42  | ALA  |
| 31  | DJ    | 81  | ILE  |
| 31  | DJ    | 94  | ALA  |
| 32  | DK    | 35  | VAL  |
| 32  | DK    | 92  | GLU  |
| 32  | DK    | 105 | ARG  |
| 32  | DK    | 108 | ARG  |
| 32  | DK    | 120 | PRO  |
| 33  | DL    | 39  | LYS  |
| 33  | DL    | 111 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 34  | DM    | 3   | GLN  |
| 35  | DN    | 70  | THR  |
| 35  | DN    | 88  | ALA  |
| 35  | DN    | 104 | ALA  |
| 35  | DN    | 107 | ASN  |
| 36  | DO    | 12  | THR  |
| 36  | DO    | 34  | HIS  |
| 36  | DO    | 57  | ALA  |
| 37  | DP    | 66  | ASN  |
| 37  | DP    | 94  | LYS  |
| 39  | DR    | 102 | SER  |
| 40  | DS    | 29  | VAL  |
| 40  | DS    | 62  | ASP  |
| 40  | DS    | 67  | ASP  |
| 40  | DS    | 72  | THR  |
| 41  | DT    | 18  | GLU  |
| 41  | DT    | 21  | SER  |
| 41  | DT    | 22  | THR  |
| 41  | DT    | 28  | ASN  |
| 41  | DT    | 39  | THR  |
| 41  | DT    | 78  | SER  |
| 42  | DU    | 37  | GLU  |
| 42  | DU    | 89  | ASP  |
| 47  | DZ    | 52  | SER  |
| 47  | DZ    | 53  | PHE  |
| 48  | D0    | 56  | ALA  |
| 49  | D1    | 16  | GLY  |
| 50  | D2    | 44  | VAL  |
| 52  | D4    | 23  | ILE  |
| 2   | AB    | 13  | GLY  |
| 2   | AB    | 20  | THR  |
| 2   | AB    | 35  | ARG  |
| 2   | AB    | 43  | LEU  |
| 2   | AB    | 80  | VAL  |
| 2   | AB    | 83  | ALA  |
| 2   | AB    | 137 | ARG  |
| 2   | AB    | 150 | GLY  |
| 2   | AB    | 156 | GLY  |
| 2   | AB    | 182 | PRO  |
| 2   | AB    | 188 | ASP  |
| 2   | AB    | 193 | PRO  |
| 2   | AB    | 210 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | AB    | 212 | LEU  |
| 2   | AB    | 220 | THR  |
| 3   | AC    | 30  | ALA  |
| 3   | AC    | 88  | ARG  |
| 3   | AC    | 166 | GLU  |
| 3   | AC    | 168 | TYR  |
| 4   | AD    | 17  | THR  |
| 4   | AD    | 24  | GLY  |
| 4   | AD    | 32  | CYS  |
| 4   | AD    | 34  | ILE  |
| 4   | AD    | 160 | GLU  |
| 5   | AE    | 12  | GLN  |
| 5   | AE    | 51  | GLY  |
| 5   | AE    | 88  | VAL  |
| 5   | AE    | 101 | GLU  |
| 5   | AE    | 109 | GLY  |
| 5   | AE    | 110 | ALA  |
| 5   | AE    | 137 | VAL  |
| 6   | AF    | 6   | ILE  |
| 7   | AG    | 5   | ARG  |
| 8   | AH    | 96  | MET  |
| 9   | AI    | 13  | LYS  |
| 9   | AI    | 67  | VAL  |
| 9   | AI    | 116 | VAL  |
| 10  | AJ    | 16  | ARG  |
| 10  | AJ    | 17  | LEU  |
| 10  | AJ    | 36  | VAL  |
| 10  | AJ    | 58  | ASN  |
| 10  | AJ    | 61  | ALA  |
| 10  | AJ    | 81  | GLU  |
| 10  | AJ    | 92  | LEU  |
| 11  | AK    | 14  | LYS  |
| 11  | AK    | 17  | SER  |
| 11  | AK    | 36  | ASP  |
| 11  | AK    | 55  | SER  |
| 11  | AK    | 108 | THR  |
| 11  | AK    | 128 | ARG  |
| 12  | AL    | 25  | GLU  |
| 12  | AL    | 26  | ALA  |
| 12  | AL    | 118 | GLY  |
| 13  | AM    | 4   | ILE  |
| 13  | AM    | 65  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 14  | AN    | 23  | LYS  |
| 14  | AN    | 28  | LYS  |
| 14  | AN    | 92  | GLU  |
| 15  | AO    | 3   | LEU  |
| 15  | AO    | 73  | LYS  |
| 15  | AO    | 88  | ARG  |
| 16  | AP    | 10  | GLY  |
| 16  | AP    | 11  | ALA  |
| 16  | AP    | 31  | ARG  |
| 16  | AP    | 48  | GLU  |
| 16  | AP    | 57  | ILE  |
| 17  | AQ    | 18  | GLU  |
| 17  | AQ    | 70  | THR  |
| 18  | AR    | 66  | SER  |
| 19  | AS    | 35  | SER  |
| 19  | AS    | 43  | ASN  |
| 20  | AT    | 5   | LYS  |
| 21  | AU    | 23  | CYS  |
| 21  | AU    | 27  | GLY  |
| 21  | AU    | 39  | GLU  |
| 24  | BC    | 124 | ILE  |
| 24  | BC    | 168 | ASP  |
| 24  | BC    | 265 | LYS  |
| 25  | BD    | 102 | ALA  |
| 25  | BD    | 104 | VAL  |
| 25  | BD    | 114 | LYS  |
| 27  | BF    | 85  | ILE  |
| 27  | BF    | 172 | ALA  |
| 28  | BG    | 39  | ASP  |
| 29  | BH    | 3   | VAL  |
| 29  | BH    | 11  | ASN  |
| 29  | BH    | 14  | SER  |
| 29  | BH    | 15  | LEU  |
| 29  | BH    | 66  | ASN  |
| 29  | BH    | 119 | ASN  |
| 30  | BI    | 10  | LYS  |
| 30  | BI    | 39  | CYS  |
| 30  | BI    | 58  | VAL  |
| 30  | BI    | 102 | SER  |
| 30  | BI    | 116 | ASP  |
| 30  | BI    | 138 | LEU  |
| 32  | BK    | 109 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 32  | BK    | 110 | GLU  |
| 33  | BL    | 15  | ALA  |
| 33  | BL    | 88  | GLY  |
| 35  | BN    | 118 | ARG  |
| 36  | BO    | 87  | ILE  |
| 37  | BP    | 16  | ASP  |
| 37  | BP    | 94  | LYS  |
| 37  | BP    | 105 | GLY  |
| 39  | BR    | 52  | PRO  |
| 39  | BR    | 55  | ASP  |
| 39  | BR    | 57  | GLY  |
| 40  | BS    | 63  | GLY  |
| 41  | BT    | 52  | GLU  |
| 41  | BT    | 71  | GLY  |
| 41  | BT    | 90  | GLY  |
| 42  | BU    | 8   | ASP  |
| 42  | BU    | 19  | LYS  |
| 43  | BV    | 66  | ASP  |
| 46  | BY    | 24  | GLU  |
| 46  | BY    | 35  | GLY  |
| 48  | B0    | 56  | ALA  |
| 49  | B1    | 52  | ALA  |
| 51  | B3    | 28  | ASN  |
| 53  | B5    | 37  | LYS  |
| 53  | B5    | 41  | THR  |
| 53  | B5    | 62  | THR  |
| 53  | B5    | 69  | LEU  |
| 53  | B5    | 90  | ALA  |
| 53  | B5    | 136 | GLY  |
| 53  | B5    | 217 | THR  |
| 53  | B5    | 219 | MET  |
| 2   | CB    | 22  | TYR  |
| 2   | CB    | 124 | GLY  |
| 2   | CB    | 130 | THR  |
| 2   | CB    | 193 | PRO  |
| 3   | CC    | 66  | VAL  |
| 3   | CC    | 140 | ASN  |
| 3   | CC    | 141 | ALA  |
| 3   | CC    | 174 | PRO  |
| 4   | CD    | 4   | TYR  |
| 4   | CD    | 43  | ALA  |
| 5   | CE    | 45  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | CE    | 51  | GLY  |
| 5   | CE    | 122 | ASN  |
| 5   | CE    | 155 | ALA  |
| 6   | CF    | 93  | LYS  |
| 6   | CF    | 94  | HIS  |
| 7   | CG    | 114 | LYS  |
| 8   | CH    | 54  | ASP  |
| 9   | CI    | 57  | MET  |
| 9   | CI    | 72  | ILE  |
| 9   | CI    | 123 | ARG  |
| 10  | CJ    | 38  | GLY  |
| 10  | CJ    | 41  | PRO  |
| 10  | CJ    | 57  | VAL  |
| 10  | CJ    | 90  | LEU  |
| 10  | CJ    | 93  | ALA  |
| 11  | CK    | 78  | GLY  |
| 11  | CK    | 126 | LYS  |
| 12  | CL    | 76  | GLU  |
| 13  | CM    | 94  | GLY  |
| 14  | CN    | 53  | ARG  |
| 15  | CO    | 21  | ASP  |
| 16  | CP    | 77  | GLU  |
| 17  | CQ    | 18  | GLU  |
| 19  | CS    | 6   | LYS  |
| 19  | CS    | 45  | ILE  |
| 21  | CU    | 35  | ARG  |
| 24  | DC    | 205 | LEU  |
| 24  | DC    | 239 | ASN  |
| 24  | DC    | 251 | GLN  |
| 24  | DC    | 255 | LYS  |
| 26  | DE    | 6   | LYS  |
| 26  | DE    | 18  | THR  |
| 26  | DE    | 61  | ARG  |
| 26  | DE    | 82  | GLY  |
| 26  | DE    | 86  | ALA  |
| 26  | DE    | 122 | GLU  |
| 26  | DE    | 126 | VAL  |
| 26  | DE    | 129 | PRO  |
| 26  | DE    | 145 | ASP  |
| 27  | DF    | 9   | LYS  |
| 27  | DF    | 148 | ARG  |
| 28  | DG    | 20  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 28  | DG    | 28  | GLY  |
| 28  | DG    | 127 | THR  |
| 28  | DG    | 175 | LYS  |
| 29  | DH    | 31  | VAL  |
| 29  | DH    | 77  | THR  |
| 29  | DH    | 118 | PRO  |
| 30  | DI    | 9   | VAL  |
| 30  | DI    | 106 | LEU  |
| 30  | DI    | 134 | ARG  |
| 33  | DL    | 40  | SER  |
| 33  | DL    | 53  | GLY  |
| 33  | DL    | 69  | ARG  |
| 34  | DM    | 23  | GLY  |
| 36  | DO    | 115 | LEU  |
| 37  | DP    | 36  | SER  |
| 37  | DP    | 80  | VAL  |
| 38  | DQ    | 102 | ASP  |
| 39  | DR    | 53  | PHE  |
| 40  | DS    | 40  | ASN  |
| 40  | DS    | 64  | ALA  |
| 40  | DS    | 66  | ILE  |
| 41  | DT    | 66  | LYS  |
| 41  | DT    | 90  | GLY  |
| 42  | DU    | 53  | ASN  |
| 42  | DU    | 57  | GLY  |
| 42  | DU    | 98  | SER  |
| 42  | DU    | 99  | ASN  |
| 45  | DX    | 7   | VAL  |
| 45  | DX    | 62  | LYS  |
| 46  | DY    | 37  | LEU  |
| 46  | DY    | 57  | LEU  |
| 47  | DZ    | 4   | THR  |
| 48  | D0    | 55  | ILE  |
| 50  | D2    | 8   | SER  |
| 50  | D2    | 45  | SER  |
| 51  | D3    | 26  | HIS  |
| 2   | AB    | 68  | LEU  |
| 2   | AB    | 202 | GLY  |
| 2   | AB    | 203 | ASN  |
| 3   | AC    | 13  | GLY  |
| 3   | AC    | 54  | ARG  |
| 3   | AC    | 127 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | AC    | 160 | ALA  |
| 4   | AD    | 36  | GLN  |
| 4   | AD    | 167 | LYS  |
| 4   | AD    | 169 | THR  |
| 5   | AE    | 45  | ARG  |
| 5   | AE    | 76  | LEU  |
| 5   | AE    | 78  | ASN  |
| 6   | AF    | 54  | LEU  |
| 6   | AF    | 69  | GLU  |
| 8   | AH    | 67  | GLN  |
| 8   | AH    | 88  | ARG  |
| 9   | AI    | 91  | ASP  |
| 10  | AJ    | 32  | THR  |
| 10  | AJ    | 41  | PRO  |
| 12  | AL    | 58  | THR  |
| 12  | AL    | 102 | LEU  |
| 13  | AM    | 10  | PRO  |
| 15  | AO    | 20  | ASN  |
| 16  | AP    | 49  | GLY  |
| 16  | AP    | 53  | ASP  |
| 17  | AQ    | 16  | LYS  |
| 19  | AS    | 4   | SER  |
| 19  | AS    | 9   | PRO  |
| 19  | AS    | 76  | PRO  |
| 20  | AT    | 68  | HIS  |
| 21  | AU    | 10  | GLU  |
| 25  | BD    | 105 | LYS  |
| 27  | BF    | 174 | ASP  |
| 27  | BF    | 176 | PRO  |
| 28  | BG    | 79  | VAL  |
| 29  | BH    | 9   | VAL  |
| 29  | BH    | 30  | LEU  |
| 29  | BH    | 85  | GLY  |
| 29  | BH    | 93  | SER  |
| 29  | BH    | 105 | ALA  |
| 30  | BI    | 20  | PRO  |
| 30  | BI    | 60  | THR  |
| 30  | BI    | 75  | PRO  |
| 30  | BI    | 84  | ALA  |
| 30  | BI    | 101 | ILE  |
| 31  | BJ    | 25  | LEU  |
| 31  | BJ    | 98  | GLU  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 35         | BN           | 10         | LEU         |
| 41         | BT           | 18         | GLU         |
| 41         | BT           | 72         | GLN         |
| 48         | B0           | 34         | SER         |
| 48         | B0           | 55         | ILE         |
| 53         | B5           | 79         | ALA         |
| 53         | B5           | 133        | GLY         |
| 2          | CB           | 19         | GLN         |
| 2          | CB           | 203        | ASN         |
| 3          | CC           | 64         | ILE         |
| 4          | CD           | 36         | GLN         |
| 4          | CD           | 168        | PRO         |
| 4          | CD           | 174        | ASP         |
| 5          | CE           | 12         | GLN         |
| 5          | CE           | 110        | ALA         |
| 5          | CE           | 138        | ARG         |
| 5          | CE           | 143        | GLY         |
| 5          | CE           | 150        | PRO         |
| 6          | CF           | 91         | ARG         |
| 6          | CF           | 95         | ALA         |
| 7          | CG           | 56         | LYS         |
| 7          | CG           | 126        | ASP         |
| 8          | CH           | 21         | ASN         |
| 8          | CH           | 97         | ALA         |
| 8          | CH           | 114        | ARG         |
| 9          | CI           | 12         | ARG         |
| 10         | CJ           | 79         | PRO         |
| 12         | CL           | 17         | ALA         |
| 12         | CL           | 22         | PRO         |
| 12         | CL           | 26         | ALA         |
| 12         | CL           | 43         | LYS         |
| 13         | CM           | 11         | ASP         |
| 13         | CM           | 12         | HIS         |
| 13         | CM           | 37         | ALA         |
| 13         | CM           | 66         | GLU         |
| 13         | CM           | 114        | LYS         |
| 14         | CN           | 21         | PHE         |
| 14         | CN           | 31         | ILE         |
| 16         | CP           | 46         | LYS         |
| 17         | CQ           | 20         | SER         |
| 17         | CQ           | 80         | GLU         |
| 18         | CR           | 47         | THR         |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 19  | CS    | 31  | LEU  |
| 20  | CT    | 5   | LYS  |
| 20  | CT    | 70  | ASN  |
| 21  | CU    | 10  | GLU  |
| 21  | CU    | 16  | LEU  |
| 24  | DC    | 34  | LEU  |
| 24  | DC    | 143 | ASN  |
| 24  | DC    | 240 | PHE  |
| 25  | DD    | 114 | LYS  |
| 26  | DE    | 48  | THR  |
| 26  | DE    | 127 | GLU  |
| 27  | DF    | 21  | ASN  |
| 28  | DG    | 8   | PRO  |
| 29  | DH    | 16  | GLY  |
| 29  | DH    | 40  | THR  |
| 31  | DJ    | 8   | PRO  |
| 31  | DJ    | 10  | THR  |
| 31  | DJ    | 25  | LEU  |
| 33  | DL    | 16  | GLY  |
| 33  | DL    | 30  | THR  |
| 33  | DL    | 42  | SER  |
| 33  | DL    | 54  | GLN  |
| 34  | DM    | 57  | VAL  |
| 34  | DM    | 58  | LYS  |
| 34  | DM    | 69  | PRO  |
| 35  | DN    | 59  | SER  |
| 35  | DN    | 105 | GLY  |
| 36  | DO    | 63  | LYS  |
| 36  | DO    | 116 | GLN  |
| 37  | DP    | 25  | THR  |
| 37  | DP    | 114 | LEU  |
| 42  | DU    | 7   | ARG  |
| 42  | DU    | 41  | LEU  |
| 42  | DU    | 52  | LEU  |
| 45  | DX    | 26  | LYS  |
| 45  | DX    | 44  | LYS  |
| 48  | D0    | 52  | ARG  |
| 49  | D1    | 27  | LYS  |
| 52  | D4    | 20  | ASP  |
| 2   | AB    | 143 | LYS  |
| 2   | AB    | 211 | THR  |
| 3   | AC    | 100 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | AD    | 26  | ARG  |
| 4   | AD    | 28  | ILE  |
| 5   | AE    | 24  | THR  |
| 5   | AE    | 108 | GLY  |
| 6   | AF    | 98  | GLU  |
| 7   | AG    | 77  | SER  |
| 7   | AG    | 85  | TYR  |
| 7   | AG    | 113 | ASP  |
| 8   | AH    | 11  | LEU  |
| 8   | AH    | 25  | VAL  |
| 8   | AH    | 57  | PRO  |
| 9   | AI    | 51  | PRO  |
| 10  | AJ    | 28  | THR  |
| 10  | AJ    | 42  | LEU  |
| 10  | AJ    | 75  | ASP  |
| 10  | AJ    | 91  | ASP  |
| 11  | AK    | 16  | VAL  |
| 11  | AK    | 119 | ASN  |
| 11  | AK    | 127 | ARG  |
| 12  | AL    | 61  | PHE  |
| 13  | AM    | 64  | VAL  |
| 15  | AO    | 46  | HIS  |
| 16  | AP    | 50  | THR  |
| 16  | AP    | 79  | ASN  |
| 17  | AQ    | 12  | VAL  |
| 17  | AQ    | 50  | ASN  |
| 20  | AT    | 69  | LYS  |
| 24  | BC    | 271 | ARG  |
| 26  | BE    | 5   | LEU  |
| 29  | BH    | 83  | LYS  |
| 30  | BI    | 4   | LYS  |
| 31  | BJ    | 81  | ILE  |
| 32  | BK    | 93  | GLN  |
| 32  | BK    | 119 | ALA  |
| 39  | BR    | 43  | ASN  |
| 40  | BS    | 42  | LYS  |
| 42  | BU    | 64  | ALA  |
| 43  | BV    | 55  | GLU  |
| 47  | BZ    | 3   | LYS  |
| 50  | B2    | 42  | LEU  |
| 53  | B5    | 27  | ALA  |
| 53  | B5    | 51  | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 53  | B5    | 65  | LEU  |
| 53  | B5    | 66  | PRO  |
| 53  | B5    | 148 | PHE  |
| 2   | CB    | 136 | MET  |
| 2   | CB    | 142 | GLU  |
| 4   | CD    | 23  | SER  |
| 4   | CD    | 29  | ASP  |
| 4   | CD    | 153 | SER  |
| 4   | CD    | 154 | ARG  |
| 4   | CD    | 192 | SER  |
| 7   | CG    | 79  | ARG  |
| 7   | CG    | 84  | THR  |
| 7   | CG    | 140 | ASP  |
| 8   | CH    | 66  | PHE  |
| 9   | CI    | 9   | THR  |
| 10  | CJ    | 35  | GLN  |
| 10  | CJ    | 36  | VAL  |
| 12  | CL    | 23  | ALA  |
| 12  | CL    | 24  | LEU  |
| 13  | CM    | 82  | ASP  |
| 14  | CN    | 62  | ASN  |
| 15  | CO    | 46  | HIS  |
| 16  | CP    | 15  | PRO  |
| 20  | CT    | 7   | ALA  |
| 24  | DC    | 76  | ALA  |
| 24  | DC    | 168 | ASP  |
| 24  | DC    | 247 | PRO  |
| 24  | DC    | 253 | LYS  |
| 24  | DC    | 260 | ASN  |
| 26  | DE    | 125 | SER  |
| 27  | DF    | 79  | ILE  |
| 27  | DF    | 174 | ASP  |
| 29  | DH    | 9   | VAL  |
| 30  | DI    | 22  | PRO  |
| 30  | DI    | 65  | ARG  |
| 30  | DI    | 84  | ALA  |
| 30  | DI    | 117 | MET  |
| 31  | DJ    | 127 | GLY  |
| 31  | DJ    | 128 | ASN  |
| 32  | DK    | 93  | GLN  |
| 33  | DL    | 25  | SER  |
| 33  | DL    | 36  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 34  | DM    | 79  | ALA  |
| 35  | DN    | 106 | ASP  |
| 35  | DN    | 118 | ARG  |
| 36  | DO    | 3   | LYS  |
| 37  | DP    | 32  | VAL  |
| 38  | DQ    | 87  | SER  |
| 39  | DR    | 82  | HIS  |
| 40  | DS    | 63  | GLY  |
| 42  | DU    | 58  | ILE  |
| 43  | DV    | 84  | PRO  |
| 47  | DZ    | 30  | ARG  |
| 49  | D1    | 5   | ILE  |
| 2   | AB    | 41  | ILE  |
| 2   | AB    | 207 | ILE  |
| 3   | AC    | 86  | LYS  |
| 3   | AC    | 121 | THR  |
| 3   | AC    | 159 | GLY  |
| 4   | AD    | 47  | ARG  |
| 4   | AD    | 161 | LEU  |
| 5   | AE    | 122 | ASN  |
| 6   | AF    | 62  | MET  |
| 8   | AH    | 34  | VAL  |
| 9   | AI    | 87  | LEU  |
| 10  | AJ    | 43  | PRO  |
| 14  | AN    | 44  | ALA  |
| 21  | AU    | 38  | TYR  |
| 24  | BC    | 121 | ASP  |
| 27  | BF    | 177 | PHE  |
| 28  | BG    | 12  | PRO  |
| 28  | BG    | 152 | ARG  |
| 30  | BI    | 8   | TYR  |
| 30  | BI    | 23  | PRO  |
| 33  | BL    | 29  | LYS  |
| 34  | BM    | 58  | LYS  |
| 36  | BO    | 77  | ALA  |
| 37  | BP    | 76  | THR  |
| 39  | BR    | 70  | GLU  |
| 52  | B4    | 37  | GLN  |
| 53  | B5    | 168 | LYS  |
| 53  | B5    | 171 | ALA  |
| 53  | B5    | 201 | LYS  |
| 53  | B5    | 210 | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 53  | B5    | 213 | VAL  |
| 53  | B5    | 223 | VAL  |
| 2   | CB    | 68  | LEU  |
| 2   | CB    | 127 | ASP  |
| 2   | CB    | 149 | GLY  |
| 3   | CC    | 37  | PHE  |
| 4   | CD    | 47  | ARG  |
| 4   | CD    | 85  | ASN  |
| 5   | CE    | 151 | GLU  |
| 6   | CF    | 18  | VAL  |
| 8   | CH    | 22  | LYS  |
| 8   | CH    | 96  | MET  |
| 9   | CI    | 55  | VAL  |
| 10  | CJ    | 95  | GLY  |
| 11  | CK    | 15  | GLN  |
| 13  | CM    | 14  | HIS  |
| 14  | CN    | 11  | VAL  |
| 17  | CQ    | 16  | LYS  |
| 19  | CS    | 67  | VAL  |
| 19  | CS    | 69  | HIS  |
| 19  | CS    | 76  | PRO  |
| 21  | CU    | 11  | PRO  |
| 24  | DC    | 85  | PRO  |
| 25  | DD    | 75  | ALA  |
| 25  | DD    | 194 | PRO  |
| 26  | DE    | 62  | GLN  |
| 26  | DE    | 200 | LEU  |
| 27  | DF    | 118 | SER  |
| 28  | DG    | 46  | ALA  |
| 28  | DG    | 80  | THR  |
| 28  | DG    | 158 | LYS  |
| 28  | DG    | 173 | GLU  |
| 30  | DI    | 10  | LYS  |
| 30  | DI    | 20  | PRO  |
| 32  | DK    | 48  | PRO  |
| 32  | DK    | 110 | GLU  |
| 33  | DL    | 29  | LYS  |
| 33  | DL    | 79  | LEU  |
| 34  | DM    | 77  | PRO  |
| 35  | DN    | 86  | ARG  |
| 39  | DR    | 7   | SER  |
| 39  | DR    | 81  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 42  | DU    | 102 | THR  |
| 43  | DV    | 85  | LYS  |
| 45  | DX    | 42  | SER  |
| 45  | DX    | 66  | THR  |
| 49  | D1    | 15  | ALA  |
| 49  | D1    | 51  | GLU  |
| 2   | AB    | 183 | VAL  |
| 3   | AC    | 66  | VAL  |
| 5   | AE    | 54  | ARG  |
| 5   | AE    | 98  | PRO  |
| 8   | AH    | 14  | ILE  |
| 9   | AI    | 9   | THR  |
| 9   | AI    | 88  | MET  |
| 13  | AM    | 66  | GLU  |
| 13  | AM    | 67  | GLY  |
| 20  | AT    | 82  | GLN  |
| 21  | AU    | 26  | ALA  |
| 24  | BC    | 97  | LYS  |
| 25  | BD    | 148 | GLN  |
| 26  | BE    | 44  | ARG  |
| 28  | BG    | 61  | GLY  |
| 29  | BH    | 120 | GLY  |
| 30  | BI    | 9   | VAL  |
| 35  | BN    | 119 | SER  |
| 36  | BO    | 88  | LYS  |
| 37  | BP    | 35  | GLY  |
| 38  | BQ    | 24  | TYR  |
| 42  | BU    | 98  | SER  |
| 2   | CB    | 205 | ASP  |
| 2   | CB    | 208 | ARG  |
| 3   | CC    | 84  | VAL  |
| 3   | CC    | 191 | THR  |
| 4   | CD    | 10  | LYS  |
| 9   | CI    | 39  | PHE  |
| 9   | CI    | 58  | VAL  |
| 9   | CI    | 128 | SER  |
| 10  | CJ    | 75  | ASP  |
| 11  | CK    | 80  | LYS  |
| 13  | CM    | 96  | PRO  |
| 16  | CP    | 14  | ARG  |
| 17  | CQ    | 5   | ILE  |
| 20  | CT    | 56  | PRO  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 20  | CT    | 65  | GLY  |
| 24  | DC    | 121 | ASP  |
| 26  | DE    | 80  | SER  |
| 26  | DE    | 83  | VAL  |
| 27  | DF    | 176 | PRO  |
| 30  | DI    | 61  | VAL  |
| 31  | DJ    | 85  | LYS  |
| 31  | DJ    | 95  | ARG  |
| 33  | DL    | 20  | GLY  |
| 41  | DT    | 50  | LEU  |
| 41  | DT    | 57  | VAL  |
| 43  | DV    | 24  | ASN  |
| 3   | AC    | 101 | ILE  |
| 8   | AH    | 100 | GLY  |
| 11  | AK    | 124 | PRO  |
| 28  | BG    | 100 | GLY  |
| 46  | BY    | 46  | VAL  |
| 47  | BZ    | 14  | ILE  |
| 6   | CF    | 85  | ILE  |
| 11  | CK    | 120 | GLY  |
| 14  | CN    | 34  | VAL  |
| 24  | DC    | 235 | GLY  |
| 27  | DF    | 31  | VAL  |
| 30  | DI    | 52  | GLY  |
| 31  | DJ    | 64  | VAL  |
| 32  | DK    | 72  | PRO  |
| 41  | DT    | 10  | VAL  |
| 45  | DX    | 51  | VAL  |
| 46  | DY    | 11  | VAL  |
| 50  | D2    | 38  | GLY  |
| 9   | AI    | 72  | ILE  |
| 13  | AM    | 111 | GLY  |
| 32  | BK    | 120 | PRO  |
| 11  | CK    | 92  | GLY  |
| 16  | CP    | 42  | ILE  |
| 17  | CQ    | 13  | VAL  |
| 20  | CT    | 67  | ILE  |
| 21  | CU    | 27  | GLY  |
| 26  | DE    | 149 | ILE  |
| 27  | DF    | 85  | ILE  |
| 28  | DG    | 12  | PRO  |
| 28  | DG    | 17  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 30  | DI    | 13  | VAL  |
| 31  | DJ    | 82  | GLY  |
| 33  | DL    | 46  | VAL  |
| 35  | DN    | 85  | PRO  |
| 41  | DT    | 47  | VAL  |
| 2   | AB    | 224 | GLY  |
| 4   | AD    | 139 | PRO  |
| 5   | AE    | 134 | ILE  |
| 6   | AF    | 43  | GLY  |
| 7   | AG    | 80  | VAL  |
| 9   | AI    | 24  | GLY  |
| 24  | BC    | 234 | GLY  |
| 30  | BI    | 13  | VAL  |
| 4   | CD    | 37  | ALA  |
| 9   | CI    | 104 | VAL  |
| 28  | DG    | 118 | PRO  |
| 32  | DK    | 119 | ALA  |
| 39  | DR    | 101 | ILE  |
| 42  | DU    | 47  | LYS  |
| 42  | DU    | 54  | GLN  |
| 51  | D3    | 7   | VAL  |
| 2   | AB    | 48  | PRO  |
| 5   | AE    | 105 | ILE  |
| 12  | AL    | 22  | PRO  |
| 18  | AR    | 26  | ILE  |
| 30  | BI    | 98  | VAL  |
| 4   | CD    | 167 | LYS  |
| 10  | CJ    | 42  | LEU  |
| 13  | CM    | 25  | VAL  |
| 14  | CN    | 72  | GLY  |
| 19  | CS    | 30  | PRO  |
| 24  | DC    | 228 | VAL  |
| 30  | DI    | 98  | VAL  |
| 42  | DU    | 25  | VAL  |
| 48  | D0    | 43  | ILE  |
| 11  | AK    | 91  | PRO  |
| 24  | BC    | 233 | GLY  |
| 6   | CF    | 64  | VAL  |

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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 |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 2   | AB    | 180/180 (100%) | 132 (73%) | 48 (27%) | 0           | 1  |
| 2   | CB    | 180/180 (100%) | 132 (73%) | 48 (27%) | 0           | 1  |
| 3   | AC    | 170/170 (100%) | 136 (80%) | 34 (20%) | 1           | 4  |
| 3   | CC    | 170/170 (100%) | 146 (86%) | 24 (14%) | 3           | 10 |
| 4   | AD    | 172/172 (100%) | 138 (80%) | 34 (20%) | 1           | 4  |
| 4   | CD    | 172/172 (100%) | 145 (84%) | 27 (16%) | 2           | 8  |
| 5   | AE    | 113/113 (100%) | 86 (76%)  | 27 (24%) | 0           | 2  |
| 5   | CE    | 113/113 (100%) | 84 (74%)  | 29 (26%) | 0           | 1  |
| 6   | AF    | 87/87 (100%)   | 71 (82%)  | 16 (18%) | 1           | 5  |
| 6   | CF    | 87/87 (100%)   | 60 (69%)  | 27 (31%) | 0           | 1  |
| 7   | AG    | 124/124 (100%) | 105 (85%) | 19 (15%) | 2           | 8  |
| 7   | CG    | 124/124 (100%) | 100 (81%) | 24 (19%) | 1           | 4  |
| 8   | AH    | 104/104 (100%) | 84 (81%)  | 20 (19%) | 1           | 4  |
| 8   | CH    | 104/104 (100%) | 84 (81%)  | 20 (19%) | 1           | 4  |
| 9   | AI    | 105/105 (100%) | 76 (72%)  | 29 (28%) | 0           | 1  |
| 9   | CI    | 105/105 (100%) | 90 (86%)  | 15 (14%) | 3           | 10 |
| 10  | AJ    | 86/86 (100%)   | 69 (80%)  | 17 (20%) | 1           | 4  |
| 10  | CJ    | 86/86 (100%)   | 65 (76%)  | 21 (24%) | 0           | 2  |
| 11  | AK    | 90/90 (100%)   | 75 (83%)  | 15 (17%) | 2           | 6  |
| 11  | CK    | 90/90 (100%)   | 73 (81%)  | 17 (19%) | 1           | 4  |
| 12  | AL    | 103/103 (100%) | 86 (84%)  | 17 (16%) | 2           | 7  |
| 12  | CL    | 103/103 (100%) | 83 (81%)  | 20 (19%) | 1           | 4  |
| 13  | AM    | 92/92 (100%)   | 76 (83%)  | 16 (17%) | 2           | 6  |
| 13  | CM    | 92/92 (100%)   | 75 (82%)  | 17 (18%) | 1           | 5  |
| 14  | AN    | 79/83 (95%)    | 65 (82%)  | 14 (18%) | 2           | 5  |
| 14  | CN    | 79/83 (95%)    | 71 (90%)  | 8 (10%)  | 7           | 23 |

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| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 15  | AO    | 75/76 (99%)    | 63 (84%)  | 12 (16%) | 2           | 7  |
| 15  | CO    | 75/76 (99%)    | 64 (85%)  | 11 (15%) | 3           | 9  |
| 16  | AP    | 65/65 (100%)   | 49 (75%)  | 16 (25%) | 0           | 2  |
| 16  | CP    | 65/65 (100%)   | 55 (85%)  | 10 (15%) | 2           | 8  |
| 17  | AQ    | 74/74 (100%)   | 50 (68%)  | 24 (32%) | 0           | 0  |
| 17  | CQ    | 74/74 (100%)   | 52 (70%)  | 22 (30%) | 0           | 1  |
| 18  | AR    | 48/48 (100%)   | 37 (77%)  | 11 (23%) | 1           | 2  |
| 18  | CR    | 48/48 (100%)   | 39 (81%)  | 9 (19%)  | 1           | 4  |
| 19  | AS    | 70/70 (100%)   | 54 (77%)  | 16 (23%) | 1           | 2  |
| 19  | CS    | 70/70 (100%)   | 57 (81%)  | 13 (19%) | 1           | 5  |
| 20  | AT    | 65/65 (100%)   | 51 (78%)  | 14 (22%) | 1           | 3  |
| 20  | CT    | 65/65 (100%)   | 57 (88%)  | 8 (12%)  | 4           | 14 |
| 21  | AU    | 44/44 (100%)   | 29 (66%)  | 15 (34%) | 0           | 0  |
| 21  | CU    | 44/44 (100%)   | 27 (61%)  | 17 (39%) | 0           | 0  |
| 24  | BC    | 216/216 (100%) | 189 (88%) | 27 (12%) | 4           | 14 |
| 24  | DC    | 216/216 (100%) | 194 (90%) | 22 (10%) | 7           | 22 |
| 25  | BD    | 164/164 (100%) | 147 (90%) | 17 (10%) | 7           | 21 |
| 25  | DD    | 164/164 (100%) | 147 (90%) | 17 (10%) | 7           | 21 |
| 26  | BE    | 165/165 (100%) | 138 (84%) | 27 (16%) | 2           | 7  |
| 26  | DE    | 165/165 (100%) | 139 (84%) | 26 (16%) | 2           | 8  |
| 27  | BF    | 148/148 (100%) | 115 (78%) | 33 (22%) | 1           | 3  |
| 27  | DF    | 148/148 (100%) | 121 (82%) | 27 (18%) | 1           | 5  |
| 28  | BG    | 137/137 (100%) | 120 (88%) | 17 (12%) | 4           | 14 |
| 28  | DG    | 137/137 (100%) | 114 (83%) | 23 (17%) | 2           | 6  |
| 29  | BH    | 114/114 (100%) | 88 (77%)  | 26 (23%) | 1           | 2  |
| 29  | DH    | 114/114 (100%) | 88 (77%)  | 26 (23%) | 1           | 2  |
| 30  | BI    | 109/109 (100%) | 83 (76%)  | 26 (24%) | 0           | 2  |
| 30  | DI    | 109/109 (100%) | 83 (76%)  | 26 (24%) | 0           | 2  |
| 31  | BJ    | 116/116 (100%) | 104 (90%) | 12 (10%) | 7           | 22 |
| 31  | DJ    | 116/116 (100%) | 97 (84%)  | 19 (16%) | 2           | 7  |
| 32  | BK    | 103/103 (100%) | 90 (87%)  | 13 (13%) | 4           | 13 |

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| Mol | Chain | Analysed       | Rotameric | Outliers | Percentiles |    |
|-----|-------|----------------|-----------|----------|-------------|----|
| 32  | DK    | 103/103 (100%) | 92 (89%)  | 11 (11%) | 6           | 20 |
| 33  | BL    | 102/102 (100%) | 92 (90%)  | 10 (10%) | 8           | 24 |
| 33  | DL    | 102/102 (100%) | 89 (87%)  | 13 (13%) | 4           | 13 |
| 34  | BM    | 109/109 (100%) | 100 (92%) | 9 (8%)   | 11          | 32 |
| 34  | DM    | 109/109 (100%) | 97 (89%)  | 12 (11%) | 6           | 19 |
| 35  | BN    | 100/100 (100%) | 93 (93%)  | 7 (7%)   | 15          | 41 |
| 35  | DN    | 100/100 (100%) | 77 (77%)  | 23 (23%) | 1           | 2  |
| 36  | BO    | 86/86 (100%)   | 66 (77%)  | 20 (23%) | 1           | 2  |
| 36  | DO    | 86/86 (100%)   | 69 (80%)  | 17 (20%) | 1           | 4  |
| 37  | BP    | 99/99 (100%)   | 84 (85%)  | 15 (15%) | 3           | 8  |
| 37  | DP    | 99/99 (100%)   | 90 (91%)  | 9 (9%)   | 9           | 28 |
| 38  | BQ    | 89/89 (100%)   | 78 (88%)  | 11 (12%) | 4           | 14 |
| 38  | DQ    | 89/89 (100%)   | 78 (88%)  | 11 (12%) | 4           | 14 |
| 39  | BR    | 84/84 (100%)   | 74 (88%)  | 10 (12%) | 5           | 15 |
| 39  | DR    | 84/84 (100%)   | 79 (94%)  | 5 (6%)   | 19          | 49 |
| 40  | BS    | 93/93 (100%)   | 77 (83%)  | 16 (17%) | 2           | 6  |
| 40  | DS    | 93/93 (100%)   | 82 (88%)  | 11 (12%) | 5           | 16 |
| 41  | BT    | 80/80 (100%)   | 70 (88%)  | 10 (12%) | 4           | 14 |
| 41  | DT    | 80/80 (100%)   | 69 (86%)  | 11 (14%) | 3           | 10 |
| 42  | BU    | 83/83 (100%)   | 71 (86%)  | 12 (14%) | 3           | 9  |
| 42  | DU    | 83/83 (100%)   | 68 (82%)  | 15 (18%) | 1           | 5  |
| 43  | BV    | 78/78 (100%)   | 61 (78%)  | 17 (22%) | 1           | 3  |
| 43  | DV    | 78/78 (100%)   | 65 (83%)  | 13 (17%) | 2           | 6  |
| 44  | BW    | 57/58 (98%)    | 48 (84%)  | 9 (16%)  | 2           | 8  |
| 44  | DW    | 56/58 (97%)    | 48 (86%)  | 8 (14%)  | 3           | 10 |
| 45  | BX    | 67/67 (100%)   | 59 (88%)  | 8 (12%)  | 5           | 15 |
| 45  | DX    | 67/67 (100%)   | 57 (85%)  | 10 (15%) | 3           | 9  |
| 46  | BY    | 55/55 (100%)   | 49 (89%)  | 6 (11%)  | 6           | 19 |
| 46  | DY    | 55/55 (100%)   | 42 (76%)  | 13 (24%) | 1           | 2  |
| 47  | BZ    | 48/48 (100%)   | 43 (90%)  | 5 (10%)  | 7           | 21 |
| 47  | DZ    | 48/48 (100%)   | 38 (79%)  | 10 (21%) | 1           | 3  |

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| Mol | Chain | Analysed        | Rotameric  | Outliers   | Percentiles |    |
|-----|-------|-----------------|------------|------------|-------------|----|
| 48  | B0    | 47/47 (100%)    | 43 (92%)   | 4 (8%)     | 10          | 31 |
| 48  | D0    | 47/47 (100%)    | 42 (89%)   | 5 (11%)    | 6           | 20 |
| 49  | B1    | 45/45 (100%)    | 42 (93%)   | 3 (7%)     | 16          | 43 |
| 49  | D1    | 45/45 (100%)    | 38 (84%)   | 7 (16%)    | 2           | 8  |
| 50  | B2    | 38/38 (100%)    | 34 (90%)   | 4 (10%)    | 7           | 21 |
| 50  | D2    | 38/38 (100%)    | 32 (84%)   | 6 (16%)    | 2           | 8  |
| 51  | B3    | 51/51 (100%)    | 45 (88%)   | 6 (12%)    | 5           | 16 |
| 51  | D3    | 51/51 (100%)    | 46 (90%)   | 5 (10%)    | 8           | 24 |
| 52  | B4    | 34/34 (100%)    | 32 (94%)   | 2 (6%)     | 19          | 49 |
| 52  | D4    | 34/34 (100%)    | 28 (82%)   | 6 (18%)    | 2           | 5  |
| 53  | B5    | 61/180 (34%)    | 47 (77%)   | 14 (23%)   | 1           | 2  |
| All | All   | 9386/9518 (99%) | 7782 (83%) | 1604 (17%) | 2           | 6  |

All (1604) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | AB    | 9   | MET  |
| 2   | AB    | 14  | VAL  |
| 2   | AB    | 15  | HIS  |
| 2   | AB    | 20  | THR  |
| 2   | AB    | 21  | ARG  |
| 2   | AB    | 27  | MET  |
| 2   | AB    | 30  | PHE  |
| 2   | AB    | 31  | ILE  |
| 2   | AB    | 32  | PHE  |
| 2   | AB    | 39  | HIS  |
| 2   | AB    | 41  | ILE  |
| 2   | AB    | 43  | LEU  |
| 2   | AB    | 46  | THR  |
| 2   | AB    | 50  | PHE  |
| 2   | AB    | 64  | LYS  |
| 2   | AB    | 66  | LYS  |
| 2   | AB    | 68  | LEU  |
| 2   | AB    | 85  | LEU  |
| 2   | AB    | 87  | CYS  |
| 2   | AB    | 88  | ASP  |
| 2   | AB    | 95  | ARG  |
| 2   | AB    | 100 | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | AB    | 101 | LEU  |
| 2   | AB    | 102 | THR  |
| 2   | AB    | 107 | VAL  |
| 2   | AB    | 108 | ARG  |
| 2   | AB    | 114 | LEU  |
| 2   | AB    | 122 | GLN  |
| 2   | AB    | 123 | ASP  |
| 2   | AB    | 126 | PHE  |
| 2   | AB    | 129 | LEU  |
| 2   | AB    | 130 | THR  |
| 2   | AB    | 132 | LYS  |
| 2   | AB    | 135 | LEU  |
| 2   | AB    | 148 | LEU  |
| 2   | AB    | 153 | ASP  |
| 2   | AB    | 157 | LEU  |
| 2   | AB    | 161 | LEU  |
| 2   | AB    | 164 | ILE  |
| 2   | AB    | 170 | HIS  |
| 2   | AB    | 188 | ASP  |
| 2   | AB    | 207 | ILE  |
| 2   | AB    | 208 | ARG  |
| 2   | AB    | 210 | VAL  |
| 2   | AB    | 213 | TYR  |
| 2   | AB    | 220 | THR  |
| 2   | AB    | 225 | ARG  |
| 2   | AB    | 226 | SER  |
| 3   | AC    | 3   | GLN  |
| 3   | AC    | 14  | ILE  |
| 3   | AC    | 15  | VAL  |
| 3   | AC    | 18  | TRP  |
| 3   | AC    | 19  | ASN  |
| 3   | AC    | 21  | THR  |
| 3   | AC    | 27  | LYS  |
| 3   | AC    | 28  | GLU  |
| 3   | AC    | 29  | PHE  |
| 3   | AC    | 33  | LEU  |
| 3   | AC    | 37  | PHE  |
| 3   | AC    | 38  | LYS  |
| 3   | AC    | 43  | LEU  |
| 3   | AC    | 52  | VAL  |
| 3   | AC    | 53  | SER  |
| 3   | AC    | 55  | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | AC    | 57  | ILE  |
| 3   | AC    | 59  | ARG  |
| 3   | AC    | 64  | ILE  |
| 3   | AC    | 69  | HIS  |
| 3   | AC    | 75  | ILE  |
| 3   | AC    | 86  | LYS  |
| 3   | AC    | 88  | ARG  |
| 3   | AC    | 107 | ARG  |
| 3   | AC    | 127 | ARG  |
| 3   | AC    | 131 | ARG  |
| 3   | AC    | 144 | LEU  |
| 3   | AC    | 167 | TRP  |
| 3   | AC    | 168 | TYR  |
| 3   | AC    | 185 | ASN  |
| 3   | AC    | 186 | THR  |
| 3   | AC    | 192 | THR  |
| 3   | AC    | 193 | TYR  |
| 3   | AC    | 196 | ILE  |
| 4   | AD    | 5   | LEU  |
| 4   | AD    | 13  | ARG  |
| 4   | AD    | 17  | THR  |
| 4   | AD    | 23  | SER  |
| 4   | AD    | 31  | LYS  |
| 4   | AD    | 32  | CYS  |
| 4   | AD    | 33  | LYS  |
| 4   | AD    | 34  | ILE  |
| 4   | AD    | 35  | GLU  |
| 4   | AD    | 44  | ARG  |
| 4   | AD    | 45  | LYS  |
| 4   | AD    | 56  | ARG  |
| 4   | AD    | 58  | LYS  |
| 4   | AD    | 63  | ARG  |
| 4   | AD    | 73  | ARG  |
| 4   | AD    | 83  | LYS  |
| 4   | AD    | 90  | LEU  |
| 4   | AD    | 93  | LEU  |
| 4   | AD    | 103 | TYR  |
| 4   | AD    | 104 | ARG  |
| 4   | AD    | 111 | ARG  |
| 4   | AD    | 121 | LYS  |
| 4   | AD    | 123 | ILE  |
| 4   | AD    | 132 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | AD    | 143 | VAL  |
| 4   | AD    | 153 | SER  |
| 4   | AD    | 161 | LEU  |
| 4   | AD    | 163 | GLU  |
| 4   | AD    | 173 | VAL  |
| 4   | AD    | 190 | ASP  |
| 4   | AD    | 195 | ILE  |
| 4   | AD    | 198 | HIS  |
| 4   | AD    | 205 | SER  |
| 4   | AD    | 206 | LYS  |
| 5   | AE    | 10  | GLU  |
| 5   | AE    | 14  | LYS  |
| 5   | AE    | 15  | LEU  |
| 5   | AE    | 16  | ILE  |
| 5   | AE    | 18  | VAL  |
| 5   | AE    | 21  | VAL  |
| 5   | AE    | 25  | VAL  |
| 5   | AE    | 32  | SER  |
| 5   | AE    | 36  | LEU  |
| 5   | AE    | 37  | THR  |
| 5   | AE    | 38  | VAL  |
| 5   | AE    | 60  | ILE  |
| 5   | AE    | 78  | ASN  |
| 5   | AE    | 81  | LEU  |
| 5   | AE    | 83  | HIS  |
| 5   | AE    | 85  | VAL  |
| 5   | AE    | 94  | VAL  |
| 5   | AE    | 115 | LEU  |
| 5   | AE    | 120 | VAL  |
| 5   | AE    | 124 | LEU  |
| 5   | AE    | 134 | ILE  |
| 5   | AE    | 136 | VAL  |
| 5   | AE    | 140 | THR  |
| 5   | AE    | 142 | ASP  |
| 5   | AE    | 149 | SER  |
| 5   | AE    | 153 | VAL  |
| 5   | AE    | 159 | LYS  |
| 6   | AF    | 7   | VAL  |
| 6   | AF    | 14  | GLN  |
| 6   | AF    | 15  | SER  |
| 6   | AF    | 17  | GLN  |
| 6   | AF    | 24  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | AF    | 50  | PRO  |
| 6   | AF    | 51  | ILE  |
| 6   | AF    | 54  | LEU  |
| 6   | AF    | 55  | HIS  |
| 6   | AF    | 68  | GLN  |
| 6   | AF    | 69  | GLU  |
| 6   | AF    | 73  | GLU  |
| 6   | AF    | 75  | GLU  |
| 6   | AF    | 84  | VAL  |
| 6   | AF    | 86  | ARG  |
| 6   | AF    | 98  | GLU  |
| 7   | AG    | 4   | ARG  |
| 7   | AG    | 7   | ILE  |
| 7   | AG    | 23  | LEU  |
| 7   | AG    | 32  | VAL  |
| 7   | AG    | 36  | LYS  |
| 7   | AG    | 38  | THR  |
| 7   | AG    | 40  | GLU  |
| 7   | AG    | 48  | GLU  |
| 7   | AG    | 50  | LEU  |
| 7   | AG    | 52  | GLN  |
| 7   | AG    | 58  | GLU  |
| 7   | AG    | 59  | LEU  |
| 7   | AG    | 63  | GLU  |
| 7   | AG    | 70  | ARG  |
| 7   | AG    | 78  | ARG  |
| 7   | AG    | 115 | SER  |
| 7   | AG    | 135 | VAL  |
| 7   | AG    | 136 | LYS  |
| 7   | AG    | 143 | ARG  |
| 8   | AH    | 2   | SER  |
| 8   | AH    | 3   | MET  |
| 8   | AH    | 22  | LYS  |
| 8   | AH    | 25  | VAL  |
| 8   | AH    | 26  | THR  |
| 8   | AH    | 36  | ILE  |
| 8   | AH    | 38  | ASN  |
| 8   | AH    | 39  | VAL  |
| 8   | AH    | 42  | GLU  |
| 8   | AH    | 47  | GLU  |
| 8   | AH    | 51  | VAL  |
| 8   | AH    | 59  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 8   | AH    | 77  | ARG  |
| 8   | AH    | 83  | LEU  |
| 8   | AH    | 87  | LYS  |
| 8   | AH    | 104 | VAL  |
| 8   | AH    | 108 | LYS  |
| 8   | AH    | 117 | ARG  |
| 8   | AH    | 121 | LEU  |
| 8   | AH    | 129 | VAL  |
| 9   | AI    | 12  | ARG  |
| 9   | AI    | 18  | ARG  |
| 9   | AI    | 30  | ILE  |
| 9   | AI    | 33  | ARG  |
| 9   | AI    | 36  | GLU  |
| 9   | AI    | 43  | THR  |
| 9   | AI    | 45  | ARG  |
| 9   | AI    | 46  | MET  |
| 9   | AI    | 47  | VAL  |
| 9   | AI    | 48  | VAL  |
| 9   | AI    | 49  | ARG  |
| 9   | AI    | 55  | VAL  |
| 9   | AI    | 56  | ASP  |
| 9   | AI    | 57  | MET  |
| 9   | AI    | 60  | LYS  |
| 9   | AI    | 61  | LEU  |
| 9   | AI    | 63  | LEU  |
| 9   | AI    | 65  | ILE  |
| 9   | AI    | 68  | LYS  |
| 9   | AI    | 85  | ARG  |
| 9   | AI    | 88  | MET  |
| 9   | AI    | 89  | GLU  |
| 9   | AI    | 90  | TYR  |
| 9   | AI    | 91  | ASP  |
| 9   | AI    | 94  | LEU  |
| 9   | AI    | 100 | LYS  |
| 9   | AI    | 127 | PHE  |
| 9   | AI    | 129 | LYS  |
| 9   | AI    | 130 | ARG  |
| 10  | AJ    | 5   | ARG  |
| 10  | AJ    | 6   | ILE  |
| 10  | AJ    | 8   | ILE  |
| 10  | AJ    | 27  | GLU  |
| 10  | AJ    | 30  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10  | AJ    | 40  | ILE  |
| 10  | AJ    | 42  | LEU  |
| 10  | AJ    | 45  | ARG  |
| 10  | AJ    | 49  | PHE  |
| 10  | AJ    | 50  | THR  |
| 10  | AJ    | 52  | LEU  |
| 10  | AJ    | 59  | LYS  |
| 10  | AJ    | 66  | GLU  |
| 10  | AJ    | 73  | LEU  |
| 10  | AJ    | 84  | VAL  |
| 10  | AJ    | 87  | LEU  |
| 10  | AJ    | 91  | ASP  |
| 11  | AK    | 31  | ILE  |
| 11  | AK    | 33  | THR  |
| 11  | AK    | 34  | ILE  |
| 11  | AK    | 52  | PHE  |
| 11  | AK    | 56  | ARG  |
| 11  | AK    | 65  | VAL  |
| 11  | AK    | 81  | ASN  |
| 11  | AK    | 85  | MET  |
| 11  | AK    | 96  | THR  |
| 11  | AK    | 97  | ILE  |
| 11  | AK    | 100 | LEU  |
| 11  | AK    | 101 | ASN  |
| 11  | AK    | 107 | ILE  |
| 11  | AK    | 126 | LYS  |
| 11  | AK    | 128 | ARG  |
| 12  | AL    | 7   | LEU  |
| 12  | AL    | 10  | LYS  |
| 12  | AL    | 19  | SER  |
| 12  | AL    | 29  | GLN  |
| 12  | AL    | 30  | LYS  |
| 12  | AL    | 33  | VAL  |
| 12  | AL    | 36  | ARG  |
| 12  | AL    | 44  | LYS  |
| 12  | AL    | 58  | THR  |
| 12  | AL    | 62  | GLU  |
| 12  | AL    | 74  | LEU  |
| 12  | AL    | 89  | ASP  |
| 12  | AL    | 102 | LEU  |
| 12  | AL    | 105 | SER  |
| 12  | AL    | 110 | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12  | AL    | 115 | SER  |
| 12  | AL    | 121 | ARG  |
| 13  | AM    | 4   | ILE  |
| 13  | AM    | 7   | ILE  |
| 13  | AM    | 13  | LYS  |
| 13  | AM    | 16  | VAL  |
| 13  | AM    | 25  | VAL  |
| 13  | AM    | 27  | LYS  |
| 13  | AM    | 50  | GLU  |
| 13  | AM    | 59  | GLU  |
| 13  | AM    | 71  | ARG  |
| 13  | AM    | 72  | GLU  |
| 13  | AM    | 80  | LEU  |
| 13  | AM    | 82  | ASP  |
| 13  | AM    | 87  | ARG  |
| 13  | AM    | 90  | ARG  |
| 13  | AM    | 101 | ARG  |
| 13  | AM    | 104 | THR  |
| 14  | AN    | 7   | LYS  |
| 14  | AN    | 12  | LYS  |
| 14  | AN    | 14  | VAL  |
| 14  | AN    | 26  | GLU  |
| 14  | AN    | 28  | LYS  |
| 14  | AN    | 46  | LEU  |
| 14  | AN    | 49  | GLN  |
| 14  | AN    | 50  | THR  |
| 14  | AN    | 51  | LEU  |
| 14  | AN    | 59  | ARG  |
| 14  | AN    | 84  | VAL  |
| 14  | AN    | 85  | ARG  |
| 14  | AN    | 97  | LYS  |
| 14  | AN    | 98  | LYS  |
| 15  | AO    | 8   | THR  |
| 15  | AO    | 13  | SER  |
| 15  | AO    | 17  | ARG  |
| 15  | AO    | 22  | THR  |
| 15  | AO    | 35  | GLN  |
| 15  | AO    | 39  | LEU  |
| 15  | AO    | 59  | MET  |
| 15  | AO    | 67  | LEU  |
| 15  | AO    | 83  | GLU  |
| 15  | AO    | 85  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 15  | AO    | 87  | LEU  |
| 15  | AO    | 88  | ARG  |
| 16  | AP    | 1   | MET  |
| 16  | AP    | 2   | VAL  |
| 16  | AP    | 3   | THR  |
| 16  | AP    | 5   | ARG  |
| 16  | AP    | 8   | ARG  |
| 16  | AP    | 18  | GLN  |
| 16  | AP    | 19  | VAL  |
| 16  | AP    | 29  | ASN  |
| 16  | AP    | 33  | ILE  |
| 16  | AP    | 46  | LYS  |
| 16  | AP    | 51  | ARG  |
| 16  | AP    | 56  | ARG  |
| 16  | AP    | 66  | THR  |
| 16  | AP    | 68  | SER  |
| 16  | AP    | 76  | LYS  |
| 16  | AP    | 80  | LYS  |
| 17  | AQ    | 4   | LYS  |
| 17  | AQ    | 6   | ARG  |
| 17  | AQ    | 7   | THR  |
| 17  | AQ    | 8   | LEU  |
| 17  | AQ    | 13  | VAL  |
| 17  | AQ    | 14  | SER  |
| 17  | AQ    | 16  | LYS  |
| 17  | AQ    | 17  | MET  |
| 17  | AQ    | 21  | ILE  |
| 17  | AQ    | 29  | VAL  |
| 17  | AQ    | 30  | LYS  |
| 17  | AQ    | 33  | ILE  |
| 17  | AQ    | 38  | ILE  |
| 17  | AQ    | 48  | ASP  |
| 17  | AQ    | 52  | GLU  |
| 17  | AQ    | 55  | ILE  |
| 17  | AQ    | 61  | ILE  |
| 17  | AQ    | 69  | LYS  |
| 17  | AQ    | 74  | THR  |
| 17  | AQ    | 75  | LEU  |
| 17  | AQ    | 76  | VAL  |
| 17  | AQ    | 77  | ARG  |
| 17  | AQ    | 81  | LYS  |
| 17  | AQ    | 83  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 18  | AR    | 21  | ILE  |
| 18  | AR    | 25  | ASP  |
| 18  | AR    | 29  | LEU  |
| 18  | AR    | 30  | LYS  |
| 18  | AR    | 31  | ASN  |
| 18  | AR    | 33  | ILE  |
| 18  | AR    | 34  | THR  |
| 18  | AR    | 43  | ARG  |
| 18  | AR    | 55  | LEU  |
| 18  | AR    | 57  | ARG  |
| 18  | AR    | 71  | THR  |
| 19  | AS    | 6   | LYS  |
| 19  | AS    | 7   | LYS  |
| 19  | AS    | 21  | LYS  |
| 19  | AS    | 24  | GLU  |
| 19  | AS    | 27  | ASP  |
| 19  | AS    | 29  | LYS  |
| 19  | AS    | 32  | ARG  |
| 19  | AS    | 37  | ARG  |
| 19  | AS    | 41  | PHE  |
| 19  | AS    | 43  | ASN  |
| 19  | AS    | 45  | ILE  |
| 19  | AS    | 55  | ARG  |
| 19  | AS    | 56  | GLN  |
| 19  | AS    | 58  | VAL  |
| 19  | AS    | 63  | THR  |
| 19  | AS    | 65  | GLU  |
| 20  | AT    | 3   | ASN  |
| 20  | AT    | 5   | LYS  |
| 20  | AT    | 6   | SER  |
| 20  | AT    | 10  | ARG  |
| 20  | AT    | 12  | ILE  |
| 20  | AT    | 24  | ARG  |
| 20  | AT    | 34  | LYS  |
| 20  | AT    | 36  | TYR  |
| 20  | AT    | 54  | MET  |
| 20  | AT    | 67  | ILE  |
| 20  | AT    | 69  | LYS  |
| 20  | AT    | 70  | ASN  |
| 20  | AT    | 74  | ARG  |
| 20  | AT    | 86  | LEU  |
| 21  | AU    | 5   | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 21  | AU    | 10  | GLU  |
| 21  | AU    | 12  | PHE  |
| 21  | AU    | 18  | ARG  |
| 21  | AU    | 20  | LYS  |
| 21  | AU    | 23  | CYS  |
| 21  | AU    | 25  | LYS  |
| 21  | AU    | 28  | VAL  |
| 21  | AU    | 34  | ARG  |
| 21  | AU    | 37  | PHE  |
| 21  | AU    | 42  | THR  |
| 21  | AU    | 46  | LYS  |
| 21  | AU    | 47  | ARG  |
| 21  | AU    | 49  | LYS  |
| 21  | AU    | 54  | LYS  |
| 24  | BC    | 13  | ARG  |
| 24  | BC    | 14  | ARG  |
| 24  | BC    | 18  | LYS  |
| 24  | BC    | 20  | VAL  |
| 24  | BC    | 24  | LEU  |
| 24  | BC    | 64  | ILE  |
| 24  | BC    | 86  | ASN  |
| 24  | BC    | 97  | LYS  |
| 24  | BC    | 105 | LEU  |
| 24  | BC    | 111 | LYS  |
| 24  | BC    | 117 | GLN  |
| 24  | BC    | 121 | ASP  |
| 24  | BC    | 156 | ARG  |
| 24  | BC    | 162 | VAL  |
| 24  | BC    | 164 | ILE  |
| 24  | BC    | 174 | LEU  |
| 24  | BC    | 177 | ARG  |
| 24  | BC    | 187 | ASP  |
| 24  | BC    | 197 | ASN  |
| 24  | BC    | 199 | GLU  |
| 24  | BC    | 213 | TRP  |
| 24  | BC    | 216 | VAL  |
| 24  | BC    | 220 | VAL  |
| 24  | BC    | 228 | VAL  |
| 24  | BC    | 245 | VAL  |
| 24  | BC    | 265 | LYS  |
| 24  | BC    | 268 | VAL  |
| 25  | BD    | 1   | MET  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 25  | BD    | 4   | LEU  |
| 25  | BD    | 13  | ARG  |
| 25  | BD    | 14  | ILE  |
| 25  | BD    | 18  | ASP  |
| 25  | BD    | 42  | ASN  |
| 25  | BD    | 58  | ASN  |
| 25  | BD    | 89  | GLU  |
| 25  | BD    | 95  | SER  |
| 25  | BD    | 97  | SER  |
| 25  | BD    | 121 | THR  |
| 25  | BD    | 129 | THR  |
| 25  | BD    | 133 | THR  |
| 25  | BD    | 145 | SER  |
| 25  | BD    | 165 | MET  |
| 25  | BD    | 174 | SER  |
| 25  | BD    | 186 | LEU  |
| 26  | BE    | 4   | VAL  |
| 26  | BE    | 5   | LEU  |
| 26  | BE    | 12  | LEU  |
| 26  | BE    | 16  | GLU  |
| 26  | BE    | 40  | ARG  |
| 26  | BE    | 44  | ARG  |
| 26  | BE    | 55  | SER  |
| 26  | BE    | 63  | LYS  |
| 26  | BE    | 74  | LYS  |
| 26  | BE    | 77  | ILE  |
| 26  | BE    | 79  | ARG  |
| 26  | BE    | 90  | GLN  |
| 26  | BE    | 93  | SER  |
| 26  | BE    | 107 | SER  |
| 26  | BE    | 108 | ILE  |
| 26  | BE    | 111 | GLU  |
| 26  | BE    | 116 | ASP  |
| 26  | BE    | 120 | VAL  |
| 26  | BE    | 126 | VAL  |
| 26  | BE    | 131 | THR  |
| 26  | BE    | 136 | GLN  |
| 26  | BE    | 149 | ILE  |
| 26  | BE    | 171 | ASP  |
| 26  | BE    | 178 | VAL  |
| 26  | BE    | 197 | GLU  |
| 26  | BE    | 198 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 26  | BE    | 200 | LEU  |
| 27  | BF    | 14  | LYS  |
| 27  | BF    | 17  | MET  |
| 27  | BF    | 18  | THR  |
| 27  | BF    | 21  | ASN  |
| 27  | BF    | 25  | VAL  |
| 27  | BF    | 34  | ILE  |
| 27  | BF    | 35  | THR  |
| 27  | BF    | 36  | LEU  |
| 27  | BF    | 37  | ASN  |
| 27  | BF    | 40  | VAL  |
| 27  | BF    | 42  | GLU  |
| 27  | BF    | 44  | ILE  |
| 27  | BF    | 48  | LYS  |
| 27  | BF    | 49  | LEU  |
| 27  | BF    | 51  | ASP  |
| 27  | BF    | 67  | ILE  |
| 27  | BF    | 83  | TYR  |
| 27  | BF    | 85  | ILE  |
| 27  | BF    | 92  | ARG  |
| 27  | BF    | 104 | ILE  |
| 27  | BF    | 108 | VAL  |
| 27  | BF    | 112 | ARG  |
| 27  | BF    | 120 | LYS  |
| 27  | BF    | 125 | ARG  |
| 27  | BF    | 132 | VAL  |
| 27  | BF    | 133 | ARG  |
| 27  | BF    | 147 | ASP  |
| 27  | BF    | 150 | ARG  |
| 27  | BF    | 152 | LEU  |
| 27  | BF    | 155 | THR  |
| 27  | BF    | 158 | THR  |
| 27  | BF    | 174 | ASP  |
| 27  | BF    | 178 | ARG  |
| 28  | BG    | 11  | VAL  |
| 28  | BG    | 33  | LEU  |
| 28  | BG    | 39  | ASP  |
| 28  | BG    | 55  | ARG  |
| 28  | BG    | 56  | ASP  |
| 28  | BG    | 67  | THR  |
| 28  | BG    | 69  | ARG  |
| 28  | BG    | 77  | ILE  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 28         | BG           | 84         | THR         |
| 28         | BG           | 87         | LEU         |
| 28         | BG           | 88         | GLN         |
| 28         | BG           | 99         | LYS         |
| 28         | BG           | 104        | ASN         |
| 28         | BG           | 124        | GLU         |
| 28         | BG           | 133        | LEU         |
| 28         | BG           | 139        | GLN         |
| 28         | BG           | 155        | GLU         |
| 29         | BH           | 1          | MET         |
| 29         | BH           | 3          | VAL         |
| 29         | BH           | 6          | LEU         |
| 29         | BH           | 12         | LEU         |
| 29         | BH           | 15         | LEU         |
| 29         | BH           | 27         | ARG         |
| 29         | BH           | 50         | ARG         |
| 29         | BH           | 60         | GLU         |
| 29         | BH           | 62         | LEU         |
| 29         | BH           | 66         | ASN         |
| 29         | BH           | 75         | LEU         |
| 29         | BH           | 77         | THR         |
| 29         | BH           | 79         | THR         |
| 29         | BH           | 86         | ASP         |
| 29         | BH           | 91         | PHE         |
| 29         | BH           | 112        | LYS         |
| 29         | BH           | 119        | ASN         |
| 29         | BH           | 122        | LEU         |
| 29         | BH           | 123        | ARG         |
| 29         | BH           | 125        | THR         |
| 29         | BH           | 129        | GLU         |
| 29         | BH           | 131        | SER         |
| 29         | BH           | 137        | GLU         |
| 29         | BH           | 142        | VAL         |
| 29         | BH           | 145        | ASN         |
| 29         | BH           | 146        | VAL         |
| 30         | BI           | 3          | LYS         |
| 30         | BI           | 9          | VAL         |
| 30         | BI           | 13         | VAL         |
| 30         | BI           | 17         | MET         |
| 30         | BI           | 19         | ASN         |
| 30         | BI           | 31         | GLN         |
| 30         | BI           | 34         | ASN         |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 30  | BI    | 38  | PHE  |
| 30  | BI    | 45  | LYS  |
| 30  | BI    | 47  | ASP  |
| 30  | BI    | 50  | GLU  |
| 30  | BI    | 51  | LYS  |
| 30  | BI    | 58  | VAL  |
| 30  | BI    | 69  | PHE  |
| 30  | BI    | 72  | LYS  |
| 30  | BI    | 82  | LYS  |
| 30  | BI    | 86  | ILE  |
| 30  | BI    | 87  | LYS  |
| 30  | BI    | 90  | SER  |
| 30  | BI    | 94  | ASN  |
| 30  | BI    | 103 | ARG  |
| 30  | BI    | 107 | GLN  |
| 30  | BI    | 125 | MET  |
| 30  | BI    | 128 | SER  |
| 30  | BI    | 134 | ARG  |
| 30  | BI    | 136 | MET  |
| 31  | BJ    | 5   | THR  |
| 31  | BJ    | 30  | THR  |
| 31  | BJ    | 37  | ARG  |
| 31  | BJ    | 40  | HIS  |
| 31  | BJ    | 43  | GLU  |
| 31  | BJ    | 61  | LYS  |
| 31  | BJ    | 64  | VAL  |
| 31  | BJ    | 86  | GLN  |
| 31  | BJ    | 96  | ARG  |
| 31  | BJ    | 114 | LEU  |
| 31  | BJ    | 124 | VAL  |
| 31  | BJ    | 142 | ILE  |
| 32  | BK    | 1   | MET  |
| 32  | BK    | 40  | LYS  |
| 32  | BK    | 49  | ARG  |
| 32  | BK    | 58  | LEU  |
| 32  | BK    | 66  | LYS  |
| 32  | BK    | 80  | ASP  |
| 32  | BK    | 91  | SER  |
| 32  | BK    | 92  | GLU  |
| 32  | BK    | 105 | ARG  |
| 32  | BK    | 114 | LYS  |
| 32  | BK    | 116 | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 32  | BK    | 117 | SER  |
| 32  | BK    | 121 | GLU  |
| 33  | BL    | 19  | LEU  |
| 33  | BL    | 40  | SER  |
| 33  | BL    | 60  | ARG  |
| 33  | BL    | 82  | LEU  |
| 33  | BL    | 86  | GLU  |
| 33  | BL    | 94  | THR  |
| 33  | BL    | 100 | ILE  |
| 33  | BL    | 104 | GLN  |
| 33  | BL    | 115 | GLU  |
| 33  | BL    | 125 | LEU  |
| 34  | BM    | 20  | LEU  |
| 34  | BM    | 24  | THR  |
| 34  | BM    | 45  | GLN  |
| 34  | BM    | 55  | ARG  |
| 34  | BM    | 69  | PRO  |
| 34  | BM    | 80  | VAL  |
| 34  | BM    | 112 | LEU  |
| 34  | BM    | 115 | GLU  |
| 34  | BM    | 126 | ILE  |
| 35  | BN    | 2   | ARG  |
| 35  | BN    | 20  | MET  |
| 35  | BN    | 69  | ARG  |
| 35  | BN    | 70  | THR  |
| 35  | BN    | 95  | THR  |
| 35  | BN    | 113 | ILE  |
| 35  | BN    | 116 | VAL  |
| 36  | BO    | 2   | ASP  |
| 36  | BO    | 3   | LYS  |
| 36  | BO    | 4   | LYS  |
| 36  | BO    | 5   | SER  |
| 36  | BO    | 9   | ARG  |
| 36  | BO    | 17  | LYS  |
| 36  | BO    | 18  | LEU  |
| 36  | BO    | 24  | THR  |
| 36  | BO    | 27  | VAL  |
| 36  | BO    | 28  | VAL  |
| 36  | BO    | 31  | THR  |
| 36  | BO    | 36  | TYR  |
| 36  | BO    | 45  | SER  |
| 36  | BO    | 47  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 36  | BO    | 49  | VAL  |
| 36  | BO    | 55  | GLU  |
| 36  | BO    | 60  | GLU  |
| 36  | BO    | 61  | GLN  |
| 36  | BO    | 87  | ILE  |
| 36  | BO    | 89  | ASP  |
| 37  | BP    | 6   | LYS  |
| 37  | BP    | 7   | GLN  |
| 37  | BP    | 12  | GLN  |
| 37  | BP    | 26  | VAL  |
| 37  | BP    | 27  | GLU  |
| 37  | BP    | 38  | LYS  |
| 37  | BP    | 57  | SER  |
| 37  | BP    | 63  | LYS  |
| 37  | BP    | 64  | ILE  |
| 37  | BP    | 68  | GLU  |
| 37  | BP    | 88  | ARG  |
| 37  | BP    | 93  | ARG  |
| 37  | BP    | 103 | ARG  |
| 37  | BP    | 109 | ARG  |
| 37  | BP    | 110 | ILE  |
| 38  | BQ    | 18  | LEU  |
| 38  | BQ    | 30  | ARG  |
| 38  | BQ    | 51  | ARG  |
| 38  | BQ    | 52  | GLN  |
| 38  | BQ    | 58  | ARG  |
| 38  | BQ    | 78  | LYS  |
| 38  | BQ    | 85  | LYS  |
| 38  | BQ    | 87  | SER  |
| 38  | BQ    | 92  | ARG  |
| 38  | BQ    | 103 | LYS  |
| 38  | BQ    | 117 | LEU  |
| 39  | BR    | 10  | LYS  |
| 39  | BR    | 14  | VAL  |
| 39  | BR    | 16  | GLU  |
| 39  | BR    | 20  | VAL  |
| 39  | BR    | 32  | THR  |
| 39  | BR    | 38  | VAL  |
| 39  | BR    | 46  | GLU  |
| 39  | BR    | 48  | LYS  |
| 39  | BR    | 74  | ILE  |
| 39  | BR    | 85  | LYS  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 40         | BS           | 6          | LYS         |
| 40         | BS           | 7          | HIS         |
| 40         | BS           | 8          | ARG         |
| 40         | BS           | 19         | LEU         |
| 40         | BS           | 25         | ARG         |
| 40         | BS           | 28         | LYS         |
| 40         | BS           | 30         | SER         |
| 40         | BS           | 42         | LYS         |
| 40         | BS           | 47         | VAL         |
| 40         | BS           | 69         | LEU         |
| 40         | BS           | 81         | SER         |
| 40         | BS           | 82         | MET         |
| 40         | BS           | 90         | LYS         |
| 40         | BS           | 92         | ARG         |
| 40         | BS           | 97         | LEU         |
| 40         | BS           | 109        | ASP         |
| 41         | BT           | 1          | MET         |
| 41         | BT           | 12         | ARG         |
| 41         | BT           | 18         | GLU         |
| 41         | BT           | 27         | SER         |
| 41         | BT           | 30         | ILE         |
| 41         | BT           | 49         | LYS         |
| 41         | BT           | 70         | HIS         |
| 41         | BT           | 73         | ARG         |
| 41         | BT           | 86         | THR         |
| 41         | BT           | 93         | LEU         |
| 42         | BU           | 5          | ILE         |
| 42         | BU           | 9          | ASP         |
| 42         | BU           | 15         | THR         |
| 42         | BU           | 26         | LYS         |
| 42         | BU           | 28         | VAL         |
| 42         | BU           | 29         | LEU         |
| 42         | BU           | 52         | LEU         |
| 42         | BU           | 68         | SER         |
| 42         | BU           | 72         | ILE         |
| 42         | BU           | 77         | THR         |
| 42         | BU           | 86         | ARG         |
| 42         | BU           | 99         | ASN         |
| 43         | BV           | 1          | MET         |
| 43         | BV           | 2          | PHE         |
| 43         | BV           | 8          | VAL         |
| 43         | BV           | 10         | LYS         |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 43  | BV    | 14  | LYS  |
| 43  | BV    | 17  | SER  |
| 43  | BV    | 29  | ILE  |
| 43  | BV    | 34  | LYS  |
| 43  | BV    | 41  | GLU  |
| 43  | BV    | 43  | ASP  |
| 43  | BV    | 61  | LEU  |
| 43  | BV    | 62  | THR  |
| 43  | BV    | 65  | VAL  |
| 43  | BV    | 66  | ASP  |
| 43  | BV    | 90  | ASP  |
| 43  | BV    | 92  | VAL  |
| 43  | BV    | 93  | ARG  |
| 44  | BW    | 20  | ARG  |
| 44  | BW    | 29  | GLU  |
| 44  | BW    | 38  | VAL  |
| 44  | BW    | 39  | ARG  |
| 44  | BW    | 41  | ARG  |
| 44  | BW    | 60  | PHE  |
| 44  | BW    | 64  | ASP  |
| 44  | BW    | 72  | LYS  |
| 44  | BW    | 81  | SER  |
| 45  | BX    | 5   | CYS  |
| 45  | BX    | 14  | THR  |
| 45  | BX    | 25  | THR  |
| 45  | BX    | 26  | LYS  |
| 45  | BX    | 43  | GLU  |
| 45  | BX    | 48  | THR  |
| 45  | BX    | 66  | THR  |
| 45  | BX    | 76  | GLU  |
| 46  | BY    | 5   | GLU  |
| 46  | BY    | 6   | LEU  |
| 46  | BY    | 16  | THR  |
| 46  | BY    | 22  | LEU  |
| 46  | BY    | 29  | ARG  |
| 46  | BY    | 57  | LEU  |
| 47  | BZ    | 10  | THR  |
| 47  | BZ    | 19  | LYS  |
| 47  | BZ    | 31  | ARG  |
| 47  | BZ    | 36  | VAL  |
| 47  | BZ    | 57  | VAL  |
| 48  | B0    | 20  | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 48  | B0    | 26  | THR  |
| 48  | B0    | 36  | GLU  |
| 48  | B0    | 40  | ARG  |
| 49  | B1    | 40  | ASP  |
| 49  | B1    | 47  | VAL  |
| 49  | B1    | 51  | GLU  |
| 50  | B2    | 3   | ARG  |
| 50  | B2    | 4   | THR  |
| 50  | B2    | 21  | ARG  |
| 50  | B2    | 45  | SER  |
| 51  | B3    | 5   | LYS  |
| 51  | B3    | 16  | LYS  |
| 51  | B3    | 30  | ARG  |
| 51  | B3    | 31  | HIS  |
| 51  | B3    | 47  | LYS  |
| 51  | B3    | 55  | LEU  |
| 52  | B4    | 18  | LYS  |
| 52  | B4    | 26  | ILE  |
| 53  | B5    | 21  | TYR  |
| 53  | B5    | 23  | ILE  |
| 53  | B5    | 38  | PHE  |
| 53  | B5    | 47  | LYS  |
| 53  | B5    | 48  | LEU  |
| 53  | B5    | 51  | ASP  |
| 53  | B5    | 64  | SER  |
| 53  | B5    | 73  | VAL  |
| 53  | B5    | 76  | LEU  |
| 53  | B5    | 78  | ILE  |
| 53  | B5    | 86  | GLU  |
| 53  | B5    | 93  | ASP  |
| 53  | B5    | 94  | TYR  |
| 53  | B5    | 100 | ILE  |
| 2   | CB    | 15  | HIS  |
| 2   | CB    | 16  | PHE  |
| 2   | CB    | 20  | THR  |
| 2   | CB    | 21  | ARG  |
| 2   | CB    | 23  | TRP  |
| 2   | CB    | 26  | LYS  |
| 2   | CB    | 27  | MET  |
| 2   | CB    | 32  | PHE  |
| 2   | CB    | 40  | ILE  |
| 2   | CB    | 43  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | CB    | 49  | MET  |
| 2   | CB    | 50  | PHE  |
| 2   | CB    | 56  | GLU  |
| 2   | CB    | 63  | ARG  |
| 2   | CB    | 66  | LYS  |
| 2   | CB    | 67  | ILE  |
| 2   | CB    | 68  | LEU  |
| 2   | CB    | 73  | LYS  |
| 2   | CB    | 74  | ARG  |
| 2   | CB    | 77  | SER  |
| 2   | CB    | 80  | VAL  |
| 2   | CB    | 85  | LEU  |
| 2   | CB    | 87  | CYS  |
| 2   | CB    | 88  | ASP  |
| 2   | CB    | 94  | HIS  |
| 2   | CB    | 95  | ARG  |
| 2   | CB    | 96  | TRP  |
| 2   | CB    | 101 | LEU  |
| 2   | CB    | 106 | THR  |
| 2   | CB    | 111 | ILE  |
| 2   | CB    | 126 | PHE  |
| 2   | CB    | 130 | THR  |
| 2   | CB    | 136 | MET  |
| 2   | CB    | 148 | LEU  |
| 2   | CB    | 163 | VAL  |
| 2   | CB    | 164 | ILE  |
| 2   | CB    | 171 | ILE  |
| 2   | CB    | 174 | LYS  |
| 2   | CB    | 175 | GLU  |
| 2   | CB    | 179 | LEU  |
| 2   | CB    | 187 | VAL  |
| 2   | CB    | 205 | ASP  |
| 2   | CB    | 207 | ILE  |
| 2   | CB    | 208 | ARG  |
| 2   | CB    | 210 | VAL  |
| 2   | CB    | 213 | TYR  |
| 2   | CB    | 222 | ARG  |
| 2   | CB    | 225 | ARG  |
| 3   | CC    | 3   | GLN  |
| 3   | CC    | 16  | LYS  |
| 3   | CC    | 27  | LYS  |
| 3   | CC    | 37  | PHE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | CC    | 38  | LYS  |
| 3   | CC    | 43  | LEU  |
| 3   | CC    | 70  | THR  |
| 3   | CC    | 75  | ILE  |
| 3   | CC    | 80  | LYS  |
| 3   | CC    | 103 | ILE  |
| 3   | CC    | 107 | ARG  |
| 3   | CC    | 110 | GLU  |
| 3   | CC    | 121 | THR  |
| 3   | CC    | 131 | ARG  |
| 3   | CC    | 140 | ASN  |
| 3   | CC    | 157 | LEU  |
| 3   | CC    | 167 | TRP  |
| 3   | CC    | 168 | TYR  |
| 3   | CC    | 175 | LEU  |
| 3   | CC    | 179 | ARG  |
| 3   | CC    | 185 | ASN  |
| 3   | CC    | 186 | THR  |
| 3   | CC    | 193 | TYR  |
| 3   | CC    | 200 | VAL  |
| 4   | CD    | 5   | LEU  |
| 4   | CD    | 8   | LYS  |
| 4   | CD    | 9   | LEU  |
| 4   | CD    | 10  | LYS  |
| 4   | CD    | 30  | THR  |
| 4   | CD    | 32  | CYS  |
| 4   | CD    | 33  | LYS  |
| 4   | CD    | 48  | LEU  |
| 4   | CD    | 50  | ASP  |
| 4   | CD    | 54  | GLN  |
| 4   | CD    | 55  | LEU  |
| 4   | CD    | 56  | ARG  |
| 4   | CD    | 58  | LYS  |
| 4   | CD    | 59  | GLN  |
| 4   | CD    | 81  | ARG  |
| 4   | CD    | 142 | VAL  |
| 4   | CD    | 148 | LYS  |
| 4   | CD    | 152 | GLN  |
| 4   | CD    | 155 | VAL  |
| 4   | CD    | 159 | LEU  |
| 4   | CD    | 161 | LEU  |
| 4   | CD    | 163 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4   | CD    | 174 | ASP  |
| 4   | CD    | 191 | LEU  |
| 4   | CD    | 192 | SER  |
| 4   | CD    | 200 | ILE  |
| 4   | CD    | 206 | LYS  |
| 5   | CE    | 10  | GLU  |
| 5   | CE    | 15  | LEU  |
| 5   | CE    | 24  | THR  |
| 5   | CE    | 25  | VAL  |
| 5   | CE    | 26  | LYS  |
| 5   | CE    | 32  | SER  |
| 5   | CE    | 45  | ARG  |
| 5   | CE    | 46  | VAL  |
| 5   | CE    | 52  | LYS  |
| 5   | CE    | 70  | ASN  |
| 5   | CE    | 81  | LEU  |
| 5   | CE    | 88  | VAL  |
| 5   | CE    | 93  | ARG  |
| 5   | CE    | 94  | VAL  |
| 5   | CE    | 100 | SER  |
| 5   | CE    | 101 | GLU  |
| 5   | CE    | 105 | ILE  |
| 5   | CE    | 114 | VAL  |
| 5   | CE    | 115 | LEU  |
| 5   | CE    | 126 | LYS  |
| 5   | CE    | 131 | THR  |
| 5   | CE    | 136 | VAL  |
| 5   | CE    | 140 | THR  |
| 5   | CE    | 146 | ASN  |
| 5   | CE    | 149 | SER  |
| 5   | CE    | 150 | PRO  |
| 5   | CE    | 151 | GLU  |
| 5   | CE    | 153 | VAL  |
| 5   | CE    | 156 | LYS  |
| 6   | CF    | 1   | MET  |
| 6   | CF    | 8   | PHE  |
| 6   | CF    | 16  | GLU  |
| 6   | CF    | 23  | GLU  |
| 6   | CF    | 24  | ARG  |
| 6   | CF    | 26  | THR  |
| 6   | CF    | 30  | THR  |
| 6   | CF    | 33  | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 6   | CF    | 35  | LYS  |
| 6   | CF    | 36  | ILE  |
| 6   | CF    | 38  | ARG  |
| 6   | CF    | 51  | ILE  |
| 6   | CF    | 53  | LYS  |
| 6   | CF    | 54  | LEU  |
| 6   | CF    | 55  | HIS  |
| 6   | CF    | 63  | ASN  |
| 6   | CF    | 64  | VAL  |
| 6   | CF    | 65  | GLU  |
| 6   | CF    | 69  | GLU  |
| 6   | CF    | 71  | ILE  |
| 6   | CF    | 74  | LEU  |
| 6   | CF    | 75  | GLU  |
| 6   | CF    | 80  | PHE  |
| 6   | CF    | 85  | ILE  |
| 6   | CF    | 87  | SER  |
| 6   | CF    | 93  | LYS  |
| 6   | CF    | 97  | THR  |
| 7   | CG    | 4   | ARG  |
| 7   | CG    | 5   | ARG  |
| 7   | CG    | 6   | VAL  |
| 7   | CG    | 7   | ILE  |
| 7   | CG    | 12  | ILE  |
| 7   | CG    | 22  | LEU  |
| 7   | CG    | 30  | LEU  |
| 7   | CG    | 43  | VAL  |
| 7   | CG    | 48  | GLU  |
| 7   | CG    | 59  | LEU  |
| 7   | CG    | 62  | PHE  |
| 7   | CG    | 64  | VAL  |
| 7   | CG    | 66  | LEU  |
| 7   | CG    | 67  | GLU  |
| 7   | CG    | 72  | THR  |
| 7   | CG    | 73  | VAL  |
| 7   | CG    | 78  | ARG  |
| 7   | CG    | 92  | ARG  |
| 7   | CG    | 94  | VAL  |
| 7   | CG    | 120 | LEU  |
| 7   | CG    | 123 | GLU  |
| 7   | CG    | 126 | ASP  |
| 7   | CG    | 140 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 7   | CG    | 142 | HIS  |
| 8   | CH    | 13  | ARG  |
| 8   | CH    | 26  | THR  |
| 8   | CH    | 32  | LEU  |
| 8   | CH    | 39  | VAL  |
| 8   | CH    | 42  | GLU  |
| 8   | CH    | 45  | PHE  |
| 8   | CH    | 48  | ASP  |
| 8   | CH    | 52  | GLU  |
| 8   | CH    | 67  | GLN  |
| 8   | CH    | 73  | GLU  |
| 8   | CH    | 74  | SER  |
| 8   | CH    | 75  | ILE  |
| 8   | CH    | 77  | ARG  |
| 8   | CH    | 83  | LEU  |
| 8   | CH    | 87  | LYS  |
| 8   | CH    | 92  | LEU  |
| 8   | CH    | 99  | LEU  |
| 8   | CH    | 112 | THR  |
| 8   | CH    | 121 | LEU  |
| 8   | CH    | 125 | ILE  |
| 9   | CI    | 9   | THR  |
| 9   | CI    | 21  | ILE  |
| 9   | CI    | 28  | ILE  |
| 9   | CI    | 36  | GLU  |
| 9   | CI    | 49  | ARG  |
| 9   | CI    | 50  | GLN  |
| 9   | CI    | 55  | VAL  |
| 9   | CI    | 61  | LEU  |
| 9   | CI    | 62  | ASP  |
| 9   | CI    | 88  | MET  |
| 9   | CI    | 89  | GLU  |
| 9   | CI    | 94  | LEU  |
| 9   | CI    | 111 | VAL  |
| 9   | CI    | 127 | PHE  |
| 9   | CI    | 129 | LYS  |
| 10  | CJ    | 7   | ARG  |
| 10  | CJ    | 9   | ARG  |
| 10  | CJ    | 16  | ARG  |
| 10  | CJ    | 17  | LEU  |
| 10  | CJ    | 22  | THR  |
| 10  | CJ    | 25  | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 10  | CJ    | 30  | LYS  |
| 10  | CJ    | 51  | VAL  |
| 10  | CJ    | 53  | ILE  |
| 10  | CJ    | 59  | LYS  |
| 10  | CJ    | 71  | LEU  |
| 10  | CJ    | 74  | VAL  |
| 10  | CJ    | 80  | THR  |
| 10  | CJ    | 83  | THR  |
| 10  | CJ    | 87  | LEU  |
| 10  | CJ    | 88  | MET  |
| 10  | CJ    | 90  | LEU  |
| 10  | CJ    | 91  | ASP  |
| 10  | CJ    | 100 | ILE  |
| 10  | CJ    | 101 | SER  |
| 10  | CJ    | 102 | LEU  |
| 11  | CK    | 14  | LYS  |
| 11  | CK    | 15  | GLN  |
| 11  | CK    | 26  | SER  |
| 11  | CK    | 33  | THR  |
| 11  | CK    | 64  | GLN  |
| 11  | CK    | 77  | TYR  |
| 11  | CK    | 81  | ASN  |
| 11  | CK    | 82  | LEU  |
| 11  | CK    | 83  | GLU  |
| 11  | CK    | 86  | VAL  |
| 11  | CK    | 96  | THR  |
| 11  | CK    | 106 | ARG  |
| 11  | CK    | 107 | ILE  |
| 11  | CK    | 108 | THR  |
| 11  | CK    | 109 | ASN  |
| 11  | CK    | 126 | LYS  |
| 11  | CK    | 128 | ARG  |
| 12  | CL    | 3   | THR  |
| 12  | CL    | 4   | VAL  |
| 12  | CL    | 10  | LYS  |
| 12  | CL    | 18  | LYS  |
| 12  | CL    | 19  | SER  |
| 12  | CL    | 20  | ASN  |
| 12  | CL    | 29  | GLN  |
| 12  | CL    | 38  | TYR  |
| 12  | CL    | 44  | LYS  |
| 12  | CL    | 59  | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12  | CL    | 63  | VAL  |
| 12  | CL    | 86  | ARG  |
| 12  | CL    | 89  | ASP  |
| 12  | CL    | 93  | VAL  |
| 12  | CL    | 94  | ARG  |
| 12  | CL    | 97  | THR  |
| 12  | CL    | 107 | VAL  |
| 12  | CL    | 110 | ARG  |
| 12  | CL    | 111 | LYS  |
| 12  | CL    | 121 | ARG  |
| 13  | CM    | 8   | ASN  |
| 13  | CM    | 13  | LYS  |
| 13  | CM    | 14  | HIS  |
| 13  | CM    | 19  | LEU  |
| 13  | CM    | 29  | ARG  |
| 13  | CM    | 31  | LYS  |
| 13  | CM    | 41  | GLU  |
| 13  | CM    | 48  | LEU  |
| 13  | CM    | 58  | ASP  |
| 13  | CM    | 59  | GLU  |
| 13  | CM    | 60  | VAL  |
| 13  | CM    | 63  | PHE  |
| 13  | CM    | 66  | GLU  |
| 13  | CM    | 90  | ARG  |
| 13  | CM    | 91  | HIS  |
| 13  | CM    | 101 | ARG  |
| 13  | CM    | 113 | ARG  |
| 14  | CN    | 10  | GLU  |
| 14  | CN    | 18  | ASP  |
| 14  | CN    | 23  | LYS  |
| 14  | CN    | 26  | GLU  |
| 14  | CN    | 28  | LYS  |
| 14  | CN    | 75  | ARG  |
| 14  | CN    | 77  | PHE  |
| 14  | CN    | 83  | LYS  |
| 15  | CO    | 6   | GLU  |
| 15  | CO    | 17  | ARG  |
| 15  | CO    | 18  | ASP  |
| 15  | CO    | 26  | GLU  |
| 15  | CO    | 35  | GLN  |
| 15  | CO    | 38  | HIS  |
| 15  | CO    | 64  | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 15  | CO    | 70  | LEU  |
| 15  | CO    | 84  | ARG  |
| 15  | CO    | 87  | LEU  |
| 15  | CO    | 88  | ARG  |
| 16  | CP    | 1   | MET  |
| 16  | CP    | 18  | GLN  |
| 16  | CP    | 20  | VAL  |
| 16  | CP    | 31  | ARG  |
| 16  | CP    | 46  | LYS  |
| 16  | CP    | 51  | ARG  |
| 16  | CP    | 55  | ASP  |
| 16  | CP    | 63  | GLN  |
| 16  | CP    | 74  | LEU  |
| 16  | CP    | 80  | LYS  |
| 17  | CQ    | 5   | ILE  |
| 17  | CQ    | 9   | GLN  |
| 17  | CQ    | 14  | SER  |
| 17  | CQ    | 17  | MET  |
| 17  | CQ    | 18  | GLU  |
| 17  | CQ    | 25  | ILE  |
| 17  | CQ    | 28  | PHE  |
| 17  | CQ    | 40  | ARG  |
| 17  | CQ    | 41  | THR  |
| 17  | CQ    | 50  | ASN  |
| 17  | CQ    | 52  | GLU  |
| 17  | CQ    | 55  | ILE  |
| 17  | CQ    | 61  | ILE  |
| 17  | CQ    | 62  | ARG  |
| 17  | CQ    | 63  | GLU  |
| 17  | CQ    | 65  | ARG  |
| 17  | CQ    | 70  | THR  |
| 17  | CQ    | 75  | LEU  |
| 17  | CQ    | 76  | VAL  |
| 17  | CQ    | 79  | VAL  |
| 17  | CQ    | 80  | GLU  |
| 17  | CQ    | 81  | LYS  |
| 18  | CR    | 21  | ILE  |
| 18  | CR    | 25  | ASP  |
| 18  | CR    | 33  | ILE  |
| 18  | CR    | 43  | ARG  |
| 18  | CR    | 45  | THR  |
| 18  | CR    | 47  | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 18  | CR    | 54  | GLN  |
| 18  | CR    | 57  | ARG  |
| 18  | CR    | 66  | SER  |
| 19  | CS    | 5   | LEU  |
| 19  | CS    | 6   | LYS  |
| 19  | CS    | 11  | ILE  |
| 19  | CS    | 13  | LEU  |
| 19  | CS    | 20  | GLU  |
| 19  | CS    | 21  | LYS  |
| 19  | CS    | 23  | VAL  |
| 19  | CS    | 27  | ASP  |
| 19  | CS    | 31  | LEU  |
| 19  | CS    | 36  | ARG  |
| 19  | CS    | 43  | ASN  |
| 19  | CS    | 49  | ILE  |
| 19  | CS    | 58  | VAL  |
| 20  | CT    | 6   | SER  |
| 20  | CT    | 8   | LYS  |
| 20  | CT    | 15  | GLU  |
| 20  | CT    | 30  | THR  |
| 20  | CT    | 36  | TYR  |
| 20  | CT    | 59  | ASP  |
| 20  | CT    | 64  | LYS  |
| 20  | CT    | 69  | LYS  |
| 21  | CU    | 5   | LYS  |
| 21  | CU    | 7   | ARG  |
| 21  | CU    | 12  | PHE  |
| 21  | CU    | 16  | LEU  |
| 21  | CU    | 18  | ARG  |
| 21  | CU    | 19  | PHE  |
| 21  | CU    | 21  | ARG  |
| 21  | CU    | 24  | GLU  |
| 21  | CU    | 25  | LYS  |
| 21  | CU    | 28  | VAL  |
| 21  | CU    | 34  | ARG  |
| 21  | CU    | 37  | PHE  |
| 21  | CU    | 38  | TYR  |
| 21  | CU    | 42  | THR  |
| 21  | CU    | 47  | ARG  |
| 21  | CU    | 53  | VAL  |
| 21  | CU    | 54  | LYS  |
| 24  | DC    | 6   | CYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 24  | DC    | 30  | PHE  |
| 24  | DC    | 63  | ARG  |
| 24  | DC    | 80  | ARG  |
| 24  | DC    | 94  | VAL  |
| 24  | DC    | 103 | TYR  |
| 24  | DC    | 111 | LYS  |
| 24  | DC    | 116 | ILE  |
| 24  | DC    | 130 | LEU  |
| 24  | DC    | 153 | GLN  |
| 24  | DC    | 156 | ARG  |
| 24  | DC    | 157 | SER  |
| 24  | DC    | 167 | ARG  |
| 24  | DC    | 175 | ARG  |
| 24  | DC    | 195 | VAL  |
| 24  | DC    | 202 | LEU  |
| 24  | DC    | 203 | ARG  |
| 24  | DC    | 229 | ASP  |
| 24  | DC    | 250 | VAL  |
| 24  | DC    | 259 | SER  |
| 24  | DC    | 262 | ARG  |
| 24  | DC    | 267 | ILE  |
| 25  | DD    | 4   | LEU  |
| 25  | DD    | 12  | THR  |
| 25  | DD    | 33  | ARG  |
| 25  | DD    | 55  | LYS  |
| 25  | DD    | 73  | VAL  |
| 25  | DD    | 77  | ARG  |
| 25  | DD    | 86  | GLU  |
| 25  | DD    | 95  | SER  |
| 25  | DD    | 103 | ASP  |
| 25  | DD    | 118 | PHE  |
| 25  | DD    | 129 | THR  |
| 25  | DD    | 138 | LEU  |
| 25  | DD    | 140 | HIS  |
| 25  | DD    | 141 | ARG  |
| 25  | DD    | 146 | ILE  |
| 25  | DD    | 170 | VAL  |
| 25  | DD    | 189 | VAL  |
| 26  | DE    | 9   | GLN  |
| 26  | DE    | 22  | ASP  |
| 26  | DE    | 40  | ARG  |
| 26  | DE    | 41  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 26  | DE    | 58  | LYS  |
| 26  | DE    | 69  | ARG  |
| 26  | DE    | 77  | ILE  |
| 26  | DE    | 78  | TRP  |
| 26  | DE    | 84  | THR  |
| 26  | DE    | 91  | ASP  |
| 26  | DE    | 105 | LEU  |
| 26  | DE    | 107 | SER  |
| 26  | DE    | 108 | ILE  |
| 26  | DE    | 118 | LEU  |
| 26  | DE    | 126 | VAL  |
| 26  | DE    | 127 | GLU  |
| 26  | DE    | 131 | THR  |
| 26  | DE    | 137 | LYS  |
| 26  | DE    | 149 | ILE  |
| 26  | DE    | 150 | THR  |
| 26  | DE    | 163 | ASN  |
| 26  | DE    | 164 | LEU  |
| 26  | DE    | 170 | ARG  |
| 26  | DE    | 173 | THR  |
| 26  | DE    | 187 | VAL  |
| 26  | DE    | 188 | MET  |
| 27  | DF    | 6   | ASP  |
| 27  | DF    | 7   | TYR  |
| 27  | DF    | 8   | TYR  |
| 27  | DF    | 14  | LYS  |
| 27  | DF    | 18  | THR  |
| 27  | DF    | 26  | MET  |
| 27  | DF    | 35  | THR  |
| 27  | DF    | 36  | LEU  |
| 27  | DF    | 38  | MET  |
| 27  | DF    | 44  | ILE  |
| 27  | DF    | 48  | LYS  |
| 27  | DF    | 52  | ASN  |
| 27  | DF    | 56  | ASP  |
| 27  | DF    | 64  | LYS  |
| 27  | DF    | 74  | VAL  |
| 27  | DF    | 78  | LYS  |
| 27  | DF    | 110 | ARG  |
| 27  | DF    | 117 | LEU  |
| 27  | DF    | 125 | ARG  |
| 27  | DF    | 132 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 27  | DF    | 140 | GLU  |
| 27  | DF    | 141 | ILE  |
| 27  | DF    | 143 | TYR  |
| 27  | DF    | 147 | ASP  |
| 27  | DF    | 150 | ARG  |
| 27  | DF    | 174 | ASP  |
| 27  | DF    | 177 | PHE  |
| 28  | DG    | 11  | VAL  |
| 28  | DG    | 24  | ILE  |
| 28  | DG    | 29  | LYS  |
| 28  | DG    | 30  | ASN  |
| 28  | DG    | 42  | GLU  |
| 28  | DG    | 45  | HIS  |
| 28  | DG    | 49  | THR  |
| 28  | DG    | 56  | ASP  |
| 28  | DG    | 62  | TRP  |
| 28  | DG    | 69  | ARG  |
| 28  | DG    | 89  | LEU  |
| 28  | DG    | 90  | VAL  |
| 28  | DG    | 92  | VAL  |
| 28  | DG    | 98  | VAL  |
| 28  | DG    | 117 | LEU  |
| 28  | DG    | 124 | GLU  |
| 28  | DG    | 127 | THR  |
| 28  | DG    | 139 | GLN  |
| 28  | DG    | 149 | ARG  |
| 28  | DG    | 151 | TYR  |
| 28  | DG    | 155 | GLU  |
| 28  | DG    | 158 | LYS  |
| 28  | DG    | 166 | ASP  |
| 29  | DH    | 7   | ASP  |
| 29  | DH    | 12  | LEU  |
| 29  | DH    | 41  | LYS  |
| 29  | DH    | 42  | LYS  |
| 29  | DH    | 48  | GLU  |
| 29  | DH    | 50  | ARG  |
| 29  | DH    | 53  | GLU  |
| 29  | DH    | 54  | LEU  |
| 29  | DH    | 57  | LYS  |
| 29  | DH    | 62  | LEU  |
| 29  | DH    | 77  | THR  |
| 29  | DH    | 78  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 29  | DH    | 87  | GLU  |
| 29  | DH    | 89  | LYS  |
| 29  | DH    | 94  | ILE  |
| 29  | DH    | 109 | GLU  |
| 29  | DH    | 114 | GLU  |
| 29  | DH    | 116 | ARG  |
| 29  | DH    | 117 | LEU  |
| 29  | DH    | 119 | ASN  |
| 29  | DH    | 121 | VAL  |
| 29  | DH    | 124 | THR  |
| 29  | DH    | 125 | THR  |
| 29  | DH    | 129 | GLU  |
| 29  | DH    | 142 | VAL  |
| 29  | DH    | 149 | GLU  |
| 30  | DI    | 3   | LYS  |
| 30  | DI    | 4   | LYS  |
| 30  | DI    | 8   | TYR  |
| 30  | DI    | 10  | LYS  |
| 30  | DI    | 11  | LEU  |
| 30  | DI    | 12  | GLN  |
| 30  | DI    | 24  | VAL  |
| 30  | DI    | 38  | PHE  |
| 30  | DI    | 40  | LYS  |
| 30  | DI    | 62  | TYR  |
| 30  | DI    | 68  | THR  |
| 30  | DI    | 69  | PHE  |
| 30  | DI    | 72  | LYS  |
| 30  | DI    | 79  | LEU  |
| 30  | DI    | 86  | ILE  |
| 30  | DI    | 87  | LYS  |
| 30  | DI    | 88  | SER  |
| 30  | DI    | 97  | LYS  |
| 30  | DI    | 98  | VAL  |
| 30  | DI    | 103 | ARG  |
| 30  | DI    | 105 | GLN  |
| 30  | DI    | 106 | LEU  |
| 30  | DI    | 112 | THR  |
| 30  | DI    | 117 | MET  |
| 30  | DI    | 122 | ILE  |
| 30  | DI    | 127 | ARG  |
| 31  | DJ    | 9   | GLU  |
| 31  | DJ    | 28  | LEU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 31  | DJ    | 39  | LYS  |
| 31  | DJ    | 40  | HIS  |
| 31  | DJ    | 43  | GLU  |
| 31  | DJ    | 44  | TYR  |
| 31  | DJ    | 50  | THR  |
| 31  | DJ    | 62  | VAL  |
| 31  | DJ    | 65  | THR  |
| 31  | DJ    | 72  | LYS  |
| 31  | DJ    | 76  | HIS  |
| 31  | DJ    | 81  | ILE  |
| 31  | DJ    | 84  | ILE  |
| 31  | DJ    | 85  | LYS  |
| 31  | DJ    | 96  | ARG  |
| 31  | DJ    | 103 | ILE  |
| 31  | DJ    | 109 | LEU  |
| 31  | DJ    | 129 | GLU  |
| 31  | DJ    | 138 | GLN  |
| 32  | DK    | 47  | ILE  |
| 32  | DK    | 49  | ARG  |
| 32  | DK    | 56  | ASP  |
| 32  | DK    | 66  | LYS  |
| 32  | DK    | 70  | ARG  |
| 32  | DK    | 87  | LEU  |
| 32  | DK    | 92  | GLU  |
| 32  | DK    | 95  | ILE  |
| 32  | DK    | 104 | THR  |
| 32  | DK    | 110 | GLU  |
| 32  | DK    | 114 | LYS  |
| 33  | DL    | 2   | ARG  |
| 33  | DL    | 21  | ARG  |
| 33  | DL    | 25  | SER  |
| 33  | DL    | 29  | LYS  |
| 33  | DL    | 48  | ARG  |
| 33  | DL    | 69  | ARG  |
| 33  | DL    | 78  | ARG  |
| 33  | DL    | 82  | LEU  |
| 33  | DL    | 94  | THR  |
| 33  | DL    | 100 | ILE  |
| 33  | DL    | 104 | GLN  |
| 33  | DL    | 118 | THR  |
| 33  | DL    | 126 | ARG  |
| 34  | DM    | 6   | ARG  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 34  | DM    | 14  | LYS  |
| 34  | DM    | 31  | PHE  |
| 34  | DM    | 47  | GLU  |
| 34  | DM    | 54  | THR  |
| 34  | DM    | 59  | ARG  |
| 34  | DM    | 60  | GLN  |
| 34  | DM    | 108 | VAL  |
| 34  | DM    | 115 | GLU  |
| 34  | DM    | 119 | LEU  |
| 34  | DM    | 124 | LEU  |
| 34  | DM    | 128 | THR  |
| 35  | DN    | 1   | MET  |
| 35  | DN    | 2   | ARG  |
| 35  | DN    | 8   | ARG  |
| 35  | DN    | 10  | LEU  |
| 35  | DN    | 12  | ARG  |
| 35  | DN    | 14  | SER  |
| 35  | DN    | 20  | MET  |
| 35  | DN    | 33  | ILE  |
| 35  | DN    | 35  | LYS  |
| 35  | DN    | 51  | LEU  |
| 35  | DN    | 53  | THR  |
| 35  | DN    | 69  | ARG  |
| 35  | DN    | 70  | THR  |
| 35  | DN    | 71  | ARG  |
| 35  | DN    | 82  | GLU  |
| 35  | DN    | 83  | LEU  |
| 35  | DN    | 90  | ARG  |
| 35  | DN    | 95  | THR  |
| 35  | DN    | 100 | CYS  |
| 35  | DN    | 114 | GLU  |
| 35  | DN    | 115 | LEU  |
| 35  | DN    | 116 | VAL  |
| 35  | DN    | 118 | ARG  |
| 36  | DO    | 5   | SER  |
| 36  | DO    | 9   | ARG  |
| 36  | DO    | 18  | LEU  |
| 36  | DO    | 26  | LEU  |
| 36  | DO    | 31  | THR  |
| 36  | DO    | 35  | ILE  |
| 36  | DO    | 36  | TYR  |
| 36  | DO    | 46  | GLU  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 36         | DO           | 47         | VAL         |
| 36         | DO           | 48         | LEU         |
| 36         | DO           | 56         | LYS         |
| 36         | DO           | 61         | GLN         |
| 36         | DO           | 78         | VAL         |
| 36         | DO           | 88         | LYS         |
| 36         | DO           | 93         | ASP         |
| 36         | DO           | 103        | VAL         |
| 36         | DO           | 117        | PHE         |
| 37         | DP           | 4          | ILE         |
| 37         | DP           | 26         | VAL         |
| 37         | DP           | 34         | GLU         |
| 37         | DP           | 68         | GLU         |
| 37         | DP           | 73         | VAL         |
| 37         | DP           | 93         | ARG         |
| 37         | DP           | 109        | ARG         |
| 37         | DP           | 110        | ILE         |
| 37         | DP           | 112        | GLU         |
| 38         | DQ           | 6          | ARG         |
| 38         | DQ           | 9          | ILE         |
| 38         | DQ           | 11         | ARG         |
| 38         | DQ           | 25         | TYR         |
| 38         | DQ           | 41         | LYS         |
| 38         | DQ           | 51         | ARG         |
| 38         | DQ           | 52         | GLN         |
| 38         | DQ           | 60         | LEU         |
| 38         | DQ           | 97         | ASP         |
| 38         | DQ           | 104        | VAL         |
| 38         | DQ           | 117        | LEU         |
| 39         | DR           | 25         | LEU         |
| 39         | DR           | 46         | GLU         |
| 39         | DR           | 48         | LYS         |
| 39         | DR           | 58         | VAL         |
| 39         | DR           | 90         | ARG         |
| 40         | DS           | 19         | LEU         |
| 40         | DS           | 20         | VAL         |
| 40         | DS           | 22         | ASP         |
| 40         | DS           | 23         | LEU         |
| 40         | DS           | 47         | VAL         |
| 40         | DS           | 57         | ASN         |
| 40         | DS           | 67         | ASP         |
| 40         | DS           | 70         | LYS         |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 40  | DS    | 72  | THR  |
| 40  | DS    | 96  | ILE  |
| 40  | DS    | 107 | VAL  |
| 41  | DT    | 3   | ARG  |
| 41  | DT    | 22  | THR  |
| 41  | DT    | 30  | ILE  |
| 41  | DT    | 32  | LEU  |
| 41  | DT    | 44  | LYS  |
| 41  | DT    | 49  | LYS  |
| 41  | DT    | 68  | LYS  |
| 41  | DT    | 69  | ARG  |
| 41  | DT    | 73  | ARG  |
| 41  | DT    | 74  | ILE  |
| 41  | DT    | 77  | ARG  |
| 42  | DU    | 11  | VAL  |
| 42  | DU    | 18  | ASP  |
| 42  | DU    | 24  | LYS  |
| 42  | DU    | 34  | VAL  |
| 42  | DU    | 35  | ILE  |
| 42  | DU    | 45  | HIS  |
| 42  | DU    | 46  | GLN  |
| 42  | DU    | 49  | VAL  |
| 42  | DU    | 54  | GLN  |
| 42  | DU    | 67  | VAL  |
| 42  | DU    | 70  | VAL  |
| 42  | DU    | 81  | ASP  |
| 42  | DU    | 85  | PHE  |
| 42  | DU    | 91  | LYS  |
| 42  | DU    | 99  | ASN  |
| 43  | DV    | 2   | PHE  |
| 43  | DV    | 3   | THR  |
| 43  | DV    | 26  | PHE  |
| 43  | DV    | 29  | ILE  |
| 43  | DV    | 30  | ILE  |
| 43  | DV    | 42  | LEU  |
| 43  | DV    | 43  | ASP  |
| 43  | DV    | 45  | ASP  |
| 43  | DV    | 50  | MET  |
| 43  | DV    | 51  | GLN  |
| 43  | DV    | 53  | LYS  |
| 43  | DV    | 65  | VAL  |
| 43  | DV    | 68  | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 44  | DW    | 20  | ARG  |
| 44  | DW    | 39  | ARG  |
| 44  | DW    | 41  | ARG  |
| 44  | DW    | 50  | ASN  |
| 44  | DW    | 56  | ASP  |
| 44  | DW    | 70  | GLU  |
| 44  | DW    | 72  | LYS  |
| 44  | DW    | 85  | GLU  |
| 45  | DX    | 4   | VAL  |
| 45  | DX    | 13  | VAL  |
| 45  | DX    | 23  | ASN  |
| 45  | DX    | 46  | PHE  |
| 45  | DX    | 47  | VAL  |
| 45  | DX    | 50  | ARG  |
| 45  | DX    | 58  | VAL  |
| 45  | DX    | 64  | ILE  |
| 45  | DX    | 71  | LEU  |
| 45  | DX    | 74  | ARG  |
| 46  | DY    | 11  | VAL  |
| 46  | DY    | 13  | GLU  |
| 46  | DY    | 16  | THR  |
| 46  | DY    | 25  | GLN  |
| 46  | DY    | 38  | GLN  |
| 46  | DY    | 39  | GLN  |
| 46  | DY    | 41  | HIS  |
| 46  | DY    | 45  | GLN  |
| 46  | DY    | 47  | ARG  |
| 46  | DY    | 49  | ASP  |
| 46  | DY    | 55  | THR  |
| 46  | DY    | 57  | LEU  |
| 46  | DY    | 58  | ASN  |
| 47  | DZ    | 3   | LYS  |
| 47  | DZ    | 6   | LYS  |
| 47  | DZ    | 10  | THR  |
| 47  | DZ    | 12  | SER  |
| 47  | DZ    | 17  | LEU  |
| 47  | DZ    | 25  | LEU  |
| 47  | DZ    | 31  | ARG  |
| 47  | DZ    | 36  | VAL  |
| 47  | DZ    | 52  | SER  |
| 47  | DZ    | 57  | VAL  |
| 48  | D0    | 3   | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 48  | D0    | 20  | ASP  |
| 48  | D0    | 22  | LEU  |
| 48  | D0    | 25  | VAL  |
| 48  | D0    | 28  | LEU  |
| 49  | D1    | 5   | ILE  |
| 49  | D1    | 12  | VAL  |
| 49  | D1    | 19  | HIS  |
| 49  | D1    | 26  | ASN  |
| 49  | D1    | 42  | VAL  |
| 49  | D1    | 46  | HIS  |
| 49  | D1    | 47  | VAL  |
| 50  | D2    | 4   | THR  |
| 50  | D2    | 10  | LEU  |
| 50  | D2    | 24  | THR  |
| 50  | D2    | 41  | ARG  |
| 50  | D2    | 43  | THR  |
| 50  | D2    | 44  | VAL  |
| 51  | D3    | 6   | THR  |
| 51  | D3    | 30  | ARG  |
| 51  | D3    | 31  | HIS  |
| 51  | D3    | 47  | LYS  |
| 51  | D3    | 49  | MET  |
| 52  | D4    | 2   | LYS  |
| 52  | D4    | 3   | VAL  |
| 52  | D4    | 12  | ARG  |
| 52  | D4    | 13  | ASN  |
| 52  | D4    | 26  | ILE  |
| 52  | D4    | 32  | LYS  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | AE    | 82  | GLN  |
| 6   | AF    | 3   | HIS  |
| 8   | AH    | 18  | GLN  |
| 9   | AI    | 126 | GLN  |
| 11  | AK    | 22  | HIS  |
| 11  | AK    | 40  | ASN  |
| 11  | AK    | 109 | ASN  |
| 13  | AM    | 91  | HIS  |
| 15  | AO    | 50  | HIS  |
| 17  | AQ    | 45  | HIS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 19  | AS    | 14  | HIS  |
| 27  | BF    | 21  | ASN  |
| 28  | BG    | 111 | HIS  |
| 29  | BH    | 119 | ASN  |
| 29  | BH    | 135 | HIS  |
| 31  | BJ    | 47  | HIS  |
| 31  | BJ    | 77  | HIS  |
| 36  | BO    | 29  | HIS  |
| 40  | BS    | 9   | HIS  |
| 53  | B5    | 45  | HIS  |
| 53  | B5    | 67  | HIS  |
| 2   | CB    | 103 | ASN  |
| 3   | CC    | 176 | HIS  |
| 4   | CD    | 136 | GLN  |
| 5   | CE    | 122 | ASN  |
| 7   | CG    | 97  | ASN  |
| 8   | CH    | 67  | GLN  |
| 9   | CI    | 25  | ASN  |
| 14  | CN    | 66  | GLN  |
| 15  | CO    | 42  | HIS  |
| 17  | CQ    | 31  | HIS  |
| 20  | CT    | 21  | ASN  |
| 20  | CT    | 61  | GLN  |
| 24  | DC    | 53  | HIS  |
| 24  | DC    | 251 | GLN  |
| 25  | DD    | 140 | HIS  |
| 25  | DD    | 150 | GLN  |
| 28  | DG    | 48  | ASN  |
| 28  | DG    | 115 | HIS  |
| 29  | DH    | 28  | ASN  |
| 29  | DH    | 128 | HIS  |
| 38  | DQ    | 37  | GLN  |
| 39  | DR    | 89  | HIS  |
| 41  | DT    | 15  | HIS  |
| 42  | DU    | 74  | ASN  |
| 45  | DX    | 34  | HIS  |
| 46  | DY    | 41  | HIS  |
| 48  | D0    | 19  | HIS  |
| 49  | D1    | 19  | HIS  |
| 49  | D1    | 26  | ASN  |
| 51  | D3    | 31  | HIS  |

## 5.3.3 RNA ⓘ

| Mol | Chain | Analysed        | Backbone Outliers | Pucker Outliers |
|-----|-------|-----------------|-------------------|-----------------|
| 1   | AA    | 1537/1539 (99%) | 327 (21%)         | 10 (0%)         |
| 1   | CA    | 1538/1539 (99%) | 330 (21%)         | 8 (0%)          |
| 22  | BA    | 2896/2903 (99%) | 569 (19%)         | 27 (0%)         |
| 22  | DA    | 2895/2903 (99%) | 685 (23%)         | 30 (1%)         |
| 23  | BB    | 118/119 (99%)   | 17 (14%)          | 0               |
| 23  | DB    | 117/119 (98%)   | 20 (17%)          | 0               |
| All | All   | 9101/9122 (99%) | 1948 (21%)        | 75 (0%)         |

All (1948) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AA    | 4   | U    |
| 1   | AA    | 5   | U    |
| 1   | AA    | 8   | A    |
| 1   | AA    | 9   | G    |
| 1   | AA    | 13  | U    |
| 1   | AA    | 32  | A    |
| 1   | AA    | 39  | G    |
| 1   | AA    | 47  | C    |
| 1   | AA    | 48  | C    |
| 1   | AA    | 50  | A    |
| 1   | AA    | 51  | A    |
| 1   | AA    | 70  | U    |
| 1   | AA    | 71  | A    |
| 1   | AA    | 72  | A    |
| 1   | AA    | 73  | C    |
| 1   | AA    | 74  | A    |
| 1   | AA    | 75  | G    |
| 1   | AA    | 76  | G    |
| 1   | AA    | 80  | A    |
| 1   | AA    | 81  | A    |
| 1   | AA    | 82  | G    |
| 1   | AA    | 83  | C    |
| 1   | AA    | 85  | U    |
| 1   | AA    | 86  | G    |
| 1   | AA    | 89  | U    |
| 1   | AA    | 90  | C    |
| 1   | AA    | 91  | U    |
| 1   | AA    | 95  | C    |
| 1   | AA    | 97  | G    |
| 1   | AA    | 108 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AA    | 116 | A    |
| 1   | AA    | 120 | A    |
| 1   | AA    | 121 | U    |
| 1   | AA    | 122 | G    |
| 1   | AA    | 127 | G    |
| 1   | AA    | 130 | A    |
| 1   | AA    | 131 | A    |
| 1   | AA    | 137 | U    |
| 1   | AA    | 138 | G    |
| 1   | AA    | 140 | U    |
| 1   | AA    | 143 | A    |
| 1   | AA    | 144 | G    |
| 1   | AA    | 163 | C    |
| 1   | AA    | 168 | G    |
| 1   | AA    | 177 | G    |
| 1   | AA    | 181 | A    |
| 1   | AA    | 182 | A    |
| 1   | AA    | 183 | C    |
| 1   | AA    | 188 | C    |
| 1   | AA    | 191 | G    |
| 1   | AA    | 195 | A    |
| 1   | AA    | 197 | A    |
| 1   | AA    | 205 | A    |
| 1   | AA    | 206 | C    |
| 1   | AA    | 210 | C    |
| 1   | AA    | 211 | G    |
| 1   | AA    | 217 | C    |
| 1   | AA    | 226 | G    |
| 1   | AA    | 240 | G    |
| 1   | AA    | 245 | U    |
| 1   | AA    | 247 | G    |
| 1   | AA    | 251 | G    |
| 1   | AA    | 262 | A    |
| 1   | AA    | 263 | A    |
| 1   | AA    | 266 | G    |
| 1   | AA    | 267 | C    |
| 1   | AA    | 281 | G    |
| 1   | AA    | 289 | G    |
| 1   | AA    | 316 | C    |
| 1   | AA    | 317 | U    |
| 1   | AA    | 318 | G    |
| 1   | AA    | 320 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AA    | 321 | A    |
| 1   | AA    | 327 | A    |
| 1   | AA    | 328 | C    |
| 1   | AA    | 329 | A    |
| 1   | AA    | 330 | C    |
| 1   | AA    | 331 | G    |
| 1   | AA    | 332 | G    |
| 1   | AA    | 346 | G    |
| 1   | AA    | 347 | G    |
| 1   | AA    | 352 | C    |
| 1   | AA    | 354 | G    |
| 1   | AA    | 364 | A    |
| 1   | AA    | 367 | U    |
| 1   | AA    | 372 | C    |
| 1   | AA    | 373 | A    |
| 1   | AA    | 376 | G    |
| 1   | AA    | 384 | G    |
| 1   | AA    | 392 | C    |
| 1   | AA    | 398 | U    |
| 1   | AA    | 406 | G    |
| 1   | AA    | 411 | A    |
| 1   | AA    | 412 | A    |
| 1   | AA    | 413 | G    |
| 1   | AA    | 414 | A    |
| 1   | AA    | 421 | U    |
| 1   | AA    | 422 | C    |
| 1   | AA    | 423 | G    |
| 1   | AA    | 429 | U    |
| 1   | AA    | 430 | A    |
| 1   | AA    | 435 | A    |
| 1   | AA    | 436 | C    |
| 1   | AA    | 445 | G    |
| 1   | AA    | 454 | G    |
| 1   | AA    | 457 | G    |
| 1   | AA    | 458 | U    |
| 1   | AA    | 462 | G    |
| 1   | AA    | 466 | A    |
| 1   | AA    | 467 | U    |
| 1   | AA    | 468 | A    |
| 1   | AA    | 476 | U    |
| 1   | AA    | 479 | U    |
| 1   | AA    | 481 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AA    | 482 | A    |
| 1   | AA    | 485 | U    |
| 1   | AA    | 486 | U    |
| 1   | AA    | 495 | A    |
| 1   | AA    | 499 | A    |
| 1   | AA    | 501 | C    |
| 1   | AA    | 505 | G    |
| 1   | AA    | 511 | C    |
| 1   | AA    | 512 | U    |
| 1   | AA    | 521 | G    |
| 1   | AA    | 524 | G    |
| 1   | AA    | 527 | G    |
| 1   | AA    | 530 | G    |
| 1   | AA    | 532 | A    |
| 1   | AA    | 533 | A    |
| 1   | AA    | 541 | G    |
| 1   | AA    | 544 | G    |
| 1   | AA    | 547 | A    |
| 1   | AA    | 559 | A    |
| 1   | AA    | 562 | U    |
| 1   | AA    | 564 | C    |
| 1   | AA    | 570 | G    |
| 1   | AA    | 573 | A    |
| 1   | AA    | 576 | C    |
| 1   | AA    | 615 | G    |
| 1   | AA    | 631 | C    |
| 1   | AA    | 632 | U    |
| 1   | AA    | 650 | G    |
| 1   | AA    | 651 | C    |
| 1   | AA    | 652 | U    |
| 1   | AA    | 653 | U    |
| 1   | AA    | 661 | G    |
| 1   | AA    | 665 | A    |
| 1   | AA    | 671 | G    |
| 1   | AA    | 686 | U    |
| 1   | AA    | 687 | A    |
| 1   | AA    | 702 | A    |
| 1   | AA    | 703 | G    |
| 1   | AA    | 721 | G    |
| 1   | AA    | 723 | U    |
| 1   | AA    | 724 | G    |
| 1   | AA    | 731 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | AA    | 748 | G    |
| 1   | AA    | 750 | C    |
| 1   | AA    | 753 | A    |
| 1   | AA    | 755 | G    |
| 1   | AA    | 765 | G    |
| 1   | AA    | 773 | G    |
| 1   | AA    | 777 | A    |
| 1   | AA    | 784 | A    |
| 1   | AA    | 792 | A    |
| 1   | AA    | 793 | U    |
| 1   | AA    | 794 | A    |
| 1   | AA    | 799 | G    |
| 1   | AA    | 814 | A    |
| 1   | AA    | 815 | A    |
| 1   | AA    | 817 | C    |
| 1   | AA    | 818 | G    |
| 1   | AA    | 828 | U    |
| 1   | AA    | 832 | G    |
| 1   | AA    | 841 | C    |
| 1   | AA    | 842 | U    |
| 1   | AA    | 843 | U    |
| 1   | AA    | 845 | A    |
| 1   | AA    | 846 | G    |
| 1   | AA    | 851 | G    |
| 1   | AA    | 859 | G    |
| 1   | AA    | 888 | G    |
| 1   | AA    | 892 | A    |
| 1   | AA    | 902 | G    |
| 1   | AA    | 910 | C    |
| 1   | AA    | 914 | A    |
| 1   | AA    | 926 | G    |
| 1   | AA    | 927 | G    |
| 1   | AA    | 934 | C    |
| 1   | AA    | 935 | A    |
| 1   | AA    | 958 | A    |
| 1   | AA    | 960 | U    |
| 1   | AA    | 966 | G    |
| 1   | AA    | 969 | A    |
| 1   | AA    | 971 | G    |
| 1   | AA    | 973 | G    |
| 1   | AA    | 975 | A    |
| 1   | AA    | 976 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | AA    | 977  | A    |
| 1   | AA    | 983  | A    |
| 1   | AA    | 987  | G    |
| 1   | AA    | 989  | U    |
| 1   | AA    | 992  | U    |
| 1   | AA    | 993  | G    |
| 1   | AA    | 1004 | A    |
| 1   | AA    | 1009 | U    |
| 1   | AA    | 1019 | A    |
| 1   | AA    | 1021 | A    |
| 1   | AA    | 1025 | U    |
| 1   | AA    | 1026 | G    |
| 1   | AA    | 1028 | C    |
| 1   | AA    | 1029 | U    |
| 1   | AA    | 1030 | U    |
| 1   | AA    | 1031 | C    |
| 1   | AA    | 1032 | G    |
| 1   | AA    | 1033 | G    |
| 1   | AA    | 1034 | G    |
| 1   | AA    | 1036 | A    |
| 1   | AA    | 1037 | C    |
| 1   | AA    | 1043 | G    |
| 1   | AA    | 1044 | A    |
| 1   | AA    | 1050 | G    |
| 1   | AA    | 1065 | U    |
| 1   | AA    | 1066 | C    |
| 1   | AA    | 1069 | C    |
| 1   | AA    | 1070 | U    |
| 1   | AA    | 1084 | G    |
| 1   | AA    | 1086 | U    |
| 1   | AA    | 1090 | U    |
| 1   | AA    | 1092 | A    |
| 1   | AA    | 1093 | A    |
| 1   | AA    | 1094 | G    |
| 1   | AA    | 1095 | U    |
| 1   | AA    | 1098 | C    |
| 1   | AA    | 1101 | A    |
| 1   | AA    | 1103 | C    |
| 1   | AA    | 1124 | G    |
| 1   | AA    | 1125 | U    |
| 1   | AA    | 1133 | G    |
| 1   | AA    | 1135 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | AA    | 1136 | C    |
| 1   | AA    | 1137 | C    |
| 1   | AA    | 1138 | G    |
| 1   | AA    | 1139 | G    |
| 1   | AA    | 1140 | C    |
| 1   | AA    | 1141 | C    |
| 1   | AA    | 1142 | G    |
| 1   | AA    | 1143 | G    |
| 1   | AA    | 1145 | A    |
| 1   | AA    | 1146 | A    |
| 1   | AA    | 1152 | A    |
| 1   | AA    | 1154 | G    |
| 1   | AA    | 1159 | U    |
| 1   | AA    | 1160 | G    |
| 1   | AA    | 1161 | C    |
| 1   | AA    | 1167 | A    |
| 1   | AA    | 1168 | U    |
| 1   | AA    | 1181 | G    |
| 1   | AA    | 1183 | U    |
| 1   | AA    | 1184 | G    |
| 1   | AA    | 1196 | A    |
| 1   | AA    | 1197 | A    |
| 1   | AA    | 1202 | U    |
| 1   | AA    | 1212 | U    |
| 1   | AA    | 1213 | A    |
| 1   | AA    | 1227 | A    |
| 1   | AA    | 1228 | C    |
| 1   | AA    | 1233 | G    |
| 1   | AA    | 1236 | A    |
| 1   | AA    | 1238 | A    |
| 1   | AA    | 1239 | A    |
| 1   | AA    | 1240 | U    |
| 1   | AA    | 1241 | G    |
| 1   | AA    | 1250 | A    |
| 1   | AA    | 1256 | A    |
| 1   | AA    | 1258 | G    |
| 1   | AA    | 1280 | A    |
| 1   | AA    | 1286 | U    |
| 1   | AA    | 1287 | A    |
| 1   | AA    | 1293 | C    |
| 1   | AA    | 1299 | A    |
| 1   | AA    | 1300 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | AA    | 1302 | C    |
| 1   | AA    | 1304 | G    |
| 1   | AA    | 1305 | G    |
| 1   | AA    | 1312 | G    |
| 1   | AA    | 1317 | C    |
| 1   | AA    | 1319 | A    |
| 1   | AA    | 1320 | C    |
| 1   | AA    | 1321 | U    |
| 1   | AA    | 1323 | G    |
| 1   | AA    | 1325 | C    |
| 1   | AA    | 1328 | C    |
| 1   | AA    | 1329 | A    |
| 1   | AA    | 1335 | U    |
| 1   | AA    | 1336 | C    |
| 1   | AA    | 1337 | G    |
| 1   | AA    | 1338 | G    |
| 1   | AA    | 1353 | G    |
| 1   | AA    | 1363 | A    |
| 1   | AA    | 1364 | U    |
| 1   | AA    | 1378 | C    |
| 1   | AA    | 1379 | G    |
| 1   | AA    | 1396 | A    |
| 1   | AA    | 1398 | A    |
| 1   | AA    | 1400 | C    |
| 1   | AA    | 1419 | G    |
| 1   | AA    | 1429 | A    |
| 1   | AA    | 1441 | A    |
| 1   | AA    | 1442 | G    |
| 1   | AA    | 1443 | C    |
| 1   | AA    | 1446 | A    |
| 1   | AA    | 1452 | C    |
| 1   | AA    | 1453 | G    |
| 1   | AA    | 1455 | G    |
| 1   | AA    | 1486 | G    |
| 1   | AA    | 1493 | A    |
| 1   | AA    | 1497 | G    |
| 1   | AA    | 1503 | A    |
| 1   | AA    | 1505 | G    |
| 1   | AA    | 1506 | U    |
| 1   | AA    | 1507 | A    |
| 1   | AA    | 1517 | G    |
| 1   | AA    | 1529 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | AA    | 1530 | G    |
| 1   | AA    | 1535 | C    |
| 1   | AA    | 1538 | C    |
| 22  | BA    | 10   | A    |
| 22  | BA    | 12   | U    |
| 22  | BA    | 13   | A    |
| 22  | BA    | 15   | G    |
| 22  | BA    | 27   | G    |
| 22  | BA    | 34   | U    |
| 22  | BA    | 35   | G    |
| 22  | BA    | 46   | G    |
| 22  | BA    | 61   | C    |
| 22  | BA    | 63   | A    |
| 22  | BA    | 71   | A    |
| 22  | BA    | 74   | A    |
| 22  | BA    | 75   | G    |
| 22  | BA    | 98   | G    |
| 22  | BA    | 118  | A    |
| 22  | BA    | 119  | A    |
| 22  | BA    | 120  | U    |
| 22  | BA    | 131  | A    |
| 22  | BA    | 138  | U    |
| 22  | BA    | 139  | U    |
| 22  | BA    | 140  | C    |
| 22  | BA    | 141  | G    |
| 22  | BA    | 142  | A    |
| 22  | BA    | 143  | C    |
| 22  | BA    | 196  | A    |
| 22  | BA    | 215  | G    |
| 22  | BA    | 216  | A    |
| 22  | BA    | 221  | A    |
| 22  | BA    | 222  | A    |
| 22  | BA    | 226  | A    |
| 22  | BA    | 248  | G    |
| 22  | BA    | 255  | A    |
| 22  | BA    | 257  | C    |
| 22  | BA    | 265  | A    |
| 22  | BA    | 266  | G    |
| 22  | BA    | 271  | G    |
| 22  | BA    | 272  | A    |
| 22  | BA    | 276  | U    |
| 22  | BA    | 279  | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 22  | BA    | 302 | C    |
| 22  | BA    | 311 | A    |
| 22  | BA    | 325 | G    |
| 22  | BA    | 329 | G    |
| 22  | BA    | 330 | A    |
| 22  | BA    | 343 | C    |
| 22  | BA    | 353 | C    |
| 22  | BA    | 361 | G    |
| 22  | BA    | 362 | A    |
| 22  | BA    | 371 | A    |
| 22  | BA    | 372 | G    |
| 22  | BA    | 386 | G    |
| 22  | BA    | 389 | G    |
| 22  | BA    | 404 | A    |
| 22  | BA    | 405 | U    |
| 22  | BA    | 411 | G    |
| 22  | BA    | 420 | C    |
| 22  | BA    | 424 | G    |
| 22  | BA    | 441 | U    |
| 22  | BA    | 450 | G    |
| 22  | BA    | 451 | U    |
| 22  | BA    | 457 | A    |
| 22  | BA    | 479 | A    |
| 22  | BA    | 481 | G    |
| 22  | BA    | 482 | A    |
| 22  | BA    | 483 | A    |
| 22  | BA    | 491 | G    |
| 22  | BA    | 501 | A    |
| 22  | BA    | 504 | A    |
| 22  | BA    | 505 | A    |
| 22  | BA    | 508 | A    |
| 22  | BA    | 528 | A    |
| 22  | BA    | 532 | A    |
| 22  | BA    | 533 | G    |
| 22  | BA    | 544 | C    |
| 22  | BA    | 546 | U    |
| 22  | BA    | 547 | A    |
| 22  | BA    | 548 | G    |
| 22  | BA    | 549 | G    |
| 22  | BA    | 563 | A    |
| 22  | BA    | 573 | U    |
| 22  | BA    | 575 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 22  | BA    | 585 | G    |
| 22  | BA    | 586 | A    |
| 22  | BA    | 603 | A    |
| 22  | BA    | 613 | A    |
| 22  | BA    | 615 | U    |
| 22  | BA    | 622 | G    |
| 22  | BA    | 627 | A    |
| 22  | BA    | 631 | A    |
| 22  | BA    | 637 | A    |
| 22  | BA    | 644 | A    |
| 22  | BA    | 645 | C    |
| 22  | BA    | 646 | U    |
| 22  | BA    | 647 | G    |
| 22  | BA    | 648 | G    |
| 22  | BA    | 653 | U    |
| 22  | BA    | 654 | A    |
| 22  | BA    | 655 | A    |
| 22  | BA    | 664 | G    |
| 22  | BA    | 669 | G    |
| 22  | BA    | 686 | U    |
| 22  | BA    | 702 | U    |
| 22  | BA    | 726 | G    |
| 22  | BA    | 729 | G    |
| 22  | BA    | 730 | A    |
| 22  | BA    | 738 | G    |
| 22  | BA    | 747 | U    |
| 22  | BA    | 749 | A    |
| 22  | BA    | 764 | A    |
| 22  | BA    | 775 | G    |
| 22  | BA    | 776 | G    |
| 22  | BA    | 782 | A    |
| 22  | BA    | 783 | A    |
| 22  | BA    | 784 | G    |
| 22  | BA    | 785 | G    |
| 22  | BA    | 790 | U    |
| 22  | BA    | 791 | C    |
| 22  | BA    | 792 | A    |
| 22  | BA    | 805 | G    |
| 22  | BA    | 812 | C    |
| 22  | BA    | 814 | C    |
| 22  | BA    | 819 | A    |
| 22  | BA    | 822 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 22  | BA    | 827  | U    |
| 22  | BA    | 828  | U    |
| 22  | BA    | 845  | A    |
| 22  | BA    | 846  | U    |
| 22  | BA    | 847  | U    |
| 22  | BA    | 858  | G    |
| 22  | BA    | 859  | G    |
| 22  | BA    | 866  | A    |
| 22  | BA    | 878  | A    |
| 22  | BA    | 879  | G    |
| 22  | BA    | 882  | G    |
| 22  | BA    | 885  | C    |
| 22  | BA    | 893  | C    |
| 22  | BA    | 896  | A    |
| 22  | BA    | 897  | C    |
| 22  | BA    | 910  | A    |
| 22  | BA    | 914  | G    |
| 22  | BA    | 915  | C    |
| 22  | BA    | 931  | U    |
| 22  | BA    | 932  | U    |
| 22  | BA    | 934  | U    |
| 22  | BA    | 941  | A    |
| 22  | BA    | 942  | G    |
| 22  | BA    | 946  | C    |
| 22  | BA    | 961  | C    |
| 22  | BA    | 962  | G    |
| 22  | BA    | 974  | G    |
| 22  | BA    | 978  | G    |
| 22  | BA    | 982  | C    |
| 22  | BA    | 983  | A    |
| 22  | BA    | 984  | A    |
| 22  | BA    | 985  | C    |
| 22  | BA    | 991  | C    |
| 22  | BA    | 995  | C    |
| 22  | BA    | 996  | A    |
| 22  | BA    | 999  | U    |
| 22  | BA    | 1005 | C    |
| 22  | BA    | 1006 | C    |
| 22  | BA    | 1012 | U    |
| 22  | BA    | 1013 | C    |
| 22  | BA    | 1022 | G    |
| 22  | BA    | 1026 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 22  | BA    | 1033 | U    |
| 22  | BA    | 1040 | A    |
| 22  | BA    | 1046 | A    |
| 22  | BA    | 1047 | G    |
| 22  | BA    | 1057 | A    |
| 22  | BA    | 1058 | U    |
| 22  | BA    | 1061 | U    |
| 22  | BA    | 1062 | G    |
| 22  | BA    | 1063 | G    |
| 22  | BA    | 1065 | U    |
| 22  | BA    | 1066 | U    |
| 22  | BA    | 1067 | A    |
| 22  | BA    | 1068 | G    |
| 22  | BA    | 1069 | A    |
| 22  | BA    | 1070 | A    |
| 22  | BA    | 1072 | C    |
| 22  | BA    | 1073 | A    |
| 22  | BA    | 1074 | G    |
| 22  | BA    | 1075 | C    |
| 22  | BA    | 1077 | A    |
| 22  | BA    | 1079 | C    |
| 22  | BA    | 1080 | A    |
| 22  | BA    | 1081 | U    |
| 22  | BA    | 1082 | U    |
| 22  | BA    | 1087 | G    |
| 22  | BA    | 1088 | A    |
| 22  | BA    | 1089 | A    |
| 22  | BA    | 1092 | C    |
| 22  | BA    | 1093 | G    |
| 22  | BA    | 1097 | U    |
| 22  | BA    | 1098 | A    |
| 22  | BA    | 1099 | G    |
| 22  | BA    | 1100 | C    |
| 22  | BA    | 1101 | U    |
| 22  | BA    | 1103 | A    |
| 22  | BA    | 1104 | C    |
| 22  | BA    | 1106 | G    |
| 22  | BA    | 1112 | G    |
| 22  | BA    | 1128 | G    |
| 22  | BA    | 1132 | U    |
| 22  | BA    | 1133 | A    |
| 22  | BA    | 1135 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 22  | BA    | 1136 | G    |
| 22  | BA    | 1138 | G    |
| 22  | BA    | 1139 | G    |
| 22  | BA    | 1141 | U    |
| 22  | BA    | 1142 | A    |
| 22  | BA    | 1168 | G    |
| 22  | BA    | 1170 | C    |
| 22  | BA    | 1171 | G    |
| 22  | BA    | 1172 | C    |
| 22  | BA    | 1174 | U    |
| 22  | BA    | 1175 | A    |
| 22  | BA    | 1176 | U    |
| 22  | BA    | 1178 | C    |
| 22  | BA    | 1179 | G    |
| 22  | BA    | 1180 | U    |
| 22  | BA    | 1186 | G    |
| 22  | BA    | 1218 | G    |
| 22  | BA    | 1230 | A    |
| 22  | BA    | 1231 | U    |
| 22  | BA    | 1238 | G    |
| 22  | BA    | 1252 | G    |
| 22  | BA    | 1253 | A    |
| 22  | BA    | 1256 | G    |
| 22  | BA    | 1266 | G    |
| 22  | BA    | 1271 | G    |
| 22  | BA    | 1272 | A    |
| 22  | BA    | 1273 | U    |
| 22  | BA    | 1275 | A    |
| 22  | BA    | 1300 | G    |
| 22  | BA    | 1301 | A    |
| 22  | BA    | 1303 | G    |
| 22  | BA    | 1305 | C    |
| 22  | BA    | 1320 | C    |
| 22  | BA    | 1325 | U    |
| 22  | BA    | 1332 | G    |
| 22  | BA    | 1348 | C    |
| 22  | BA    | 1352 | U    |
| 22  | BA    | 1355 | G    |
| 22  | BA    | 1357 | C    |
| 22  | BA    | 1359 | A    |
| 22  | BA    | 1365 | A    |
| 22  | BA    | 1374 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 22  | BA    | 1377 | G    |
| 22  | BA    | 1378 | A    |
| 22  | BA    | 1379 | U    |
| 22  | BA    | 1383 | A    |
| 22  | BA    | 1386 | C    |
| 22  | BA    | 1406 | U    |
| 22  | BA    | 1407 | G    |
| 22  | BA    | 1411 | U    |
| 22  | BA    | 1415 | U    |
| 22  | BA    | 1416 | G    |
| 22  | BA    | 1419 | A    |
| 22  | BA    | 1420 | A    |
| 22  | BA    | 1427 | A    |
| 22  | BA    | 1428 | C    |
| 22  | BA    | 1435 | G    |
| 22  | BA    | 1437 | C    |
| 22  | BA    | 1452 | G    |
| 22  | BA    | 1453 | A    |
| 22  | BA    | 1458 | U    |
| 22  | BA    | 1475 | G    |
| 22  | BA    | 1482 | G    |
| 22  | BA    | 1483 | G    |
| 22  | BA    | 1493 | C    |
| 22  | BA    | 1494 | A    |
| 22  | BA    | 1495 | A    |
| 22  | BA    | 1504 | A    |
| 22  | BA    | 1508 | A    |
| 22  | BA    | 1510 | G    |
| 22  | BA    | 1515 | A    |
| 22  | BA    | 1530 | G    |
| 22  | BA    | 1532 | A    |
| 22  | BA    | 1533 | C    |
| 22  | BA    | 1534 | U    |
| 22  | BA    | 1535 | A    |
| 22  | BA    | 1536 | C    |
| 22  | BA    | 1547 | C    |
| 22  | BA    | 1548 | A    |
| 22  | BA    | 1554 | U    |
| 22  | BA    | 1555 | G    |
| 22  | BA    | 1560 | G    |
| 22  | BA    | 1569 | A    |
| 22  | BA    | 1578 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 22  | BA    | 1579 | A    |
| 22  | BA    | 1583 | A    |
| 22  | BA    | 1584 | U    |
| 22  | BA    | 1585 | C    |
| 22  | BA    | 1593 | A    |
| 22  | BA    | 1597 | A    |
| 22  | BA    | 1606 | C    |
| 22  | BA    | 1607 | C    |
| 22  | BA    | 1608 | A    |
| 22  | BA    | 1609 | A    |
| 22  | BA    | 1610 | A    |
| 22  | BA    | 1616 | A    |
| 22  | BA    | 1632 | A    |
| 22  | BA    | 1647 | U    |
| 22  | BA    | 1648 | U    |
| 22  | BA    | 1649 | G    |
| 22  | BA    | 1652 | A    |
| 22  | BA    | 1659 | G    |
| 22  | BA    | 1674 | G    |
| 22  | BA    | 1685 | C    |
| 22  | BA    | 1688 | U    |
| 22  | BA    | 1697 | G    |
| 22  | BA    | 1714 | U    |
| 22  | BA    | 1715 | G    |
| 22  | BA    | 1718 | G    |
| 22  | BA    | 1729 | U    |
| 22  | BA    | 1730 | C    |
| 22  | BA    | 1736 | U    |
| 22  | BA    | 1738 | G    |
| 22  | BA    | 1739 | A    |
| 22  | BA    | 1744 | A    |
| 22  | BA    | 1764 | C    |
| 22  | BA    | 1773 | A    |
| 22  | BA    | 1776 | G    |
| 22  | BA    | 1786 | A    |
| 22  | BA    | 1795 | C    |
| 22  | BA    | 1800 | C    |
| 22  | BA    | 1801 | A    |
| 22  | BA    | 1808 | A    |
| 22  | BA    | 1813 | G    |
| 22  | BA    | 1816 | C    |
| 22  | BA    | 1819 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 22  | BA    | 1828 | G    |
| 22  | BA    | 1829 | A    |
| 22  | BA    | 1830 | C    |
| 22  | BA    | 1835 | G    |
| 22  | BA    | 1839 | G    |
| 22  | BA    | 1840 | G    |
| 22  | BA    | 1841 | U    |
| 22  | BA    | 1842 | G    |
| 22  | BA    | 1849 | G    |
| 22  | BA    | 1853 | A    |
| 22  | BA    | 1870 | C    |
| 22  | BA    | 1871 | A    |
| 22  | BA    | 1872 | A    |
| 22  | BA    | 1873 | G    |
| 22  | BA    | 1876 | A    |
| 22  | BA    | 1885 | A    |
| 22  | BA    | 1886 | U    |
| 22  | BA    | 1888 | G    |
| 22  | BA    | 1890 | A    |
| 22  | BA    | 1900 | A    |
| 22  | BA    | 1902 | C    |
| 22  | BA    | 1906 | G    |
| 22  | BA    | 1909 | C    |
| 22  | BA    | 1912 | A    |
| 22  | BA    | 1913 | A    |
| 22  | BA    | 1914 | C    |
| 22  | BA    | 1915 | U    |
| 22  | BA    | 1916 | A    |
| 22  | BA    | 1917 | U    |
| 22  | BA    | 1920 | C    |
| 22  | BA    | 1923 | U    |
| 22  | BA    | 1924 | C    |
| 22  | BA    | 1925 | C    |
| 22  | BA    | 1926 | U    |
| 22  | BA    | 1929 | G    |
| 22  | BA    | 1930 | G    |
| 22  | BA    | 1931 | U    |
| 22  | BA    | 1932 | A    |
| 22  | BA    | 1938 | A    |
| 22  | BA    | 1955 | U    |
| 22  | BA    | 1964 | G    |
| 22  | BA    | 1965 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 22  | BA    | 1967 | C    |
| 22  | BA    | 1970 | A    |
| 22  | BA    | 1972 | G    |
| 22  | BA    | 1986 | C    |
| 22  | BA    | 1991 | U    |
| 22  | BA    | 1992 | G    |
| 22  | BA    | 1993 | U    |
| 22  | BA    | 1995 | U    |
| 22  | BA    | 1997 | C    |
| 22  | BA    | 2018 | G    |
| 22  | BA    | 2022 | U    |
| 22  | BA    | 2023 | C    |
| 22  | BA    | 2031 | A    |
| 22  | BA    | 2033 | A    |
| 22  | BA    | 2043 | C    |
| 22  | BA    | 2051 | A    |
| 22  | BA    | 2055 | C    |
| 22  | BA    | 2056 | G    |
| 22  | BA    | 2060 | A    |
| 22  | BA    | 2061 | G    |
| 22  | BA    | 2062 | A    |
| 22  | BA    | 2064 | C    |
| 22  | BA    | 2067 | G    |
| 22  | BA    | 2069 | G    |
| 22  | BA    | 2072 | C    |
| 22  | BA    | 2092 | U    |
| 22  | BA    | 2093 | G    |
| 22  | BA    | 2097 | A    |
| 22  | BA    | 2098 | U    |
| 22  | BA    | 2099 | U    |
| 22  | BA    | 2100 | G    |
| 22  | BA    | 2102 | G    |
| 22  | BA    | 2103 | C    |
| 22  | BA    | 2106 | U    |
| 22  | BA    | 2110 | G    |
| 22  | BA    | 2111 | U    |
| 22  | BA    | 2112 | G    |
| 22  | BA    | 2113 | U    |
| 22  | BA    | 2115 | G    |
| 22  | BA    | 2116 | G    |
| 22  | BA    | 2117 | A    |
| 22  | BA    | 2118 | U    |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> |
|------------|--------------|------------|-------------|
| 22         | BA           | 2119       | A           |
| 22         | BA           | 2122       | U           |
| 22         | BA           | 2126       | A           |
| 22         | BA           | 2127       | G           |
| 22         | BA           | 2128       | G           |
| 22         | BA           | 2129       | C           |
| 22         | BA           | 2132       | U           |
| 22         | BA           | 2133       | G           |
| 22         | BA           | 2134       | A           |
| 22         | BA           | 2136       | G           |
| 22         | BA           | 2138       | G           |
| 22         | BA           | 2139       | U           |
| 22         | BA           | 2145       | C           |
| 22         | BA           | 2147       | A           |
| 22         | BA           | 2148       | G           |
| 22         | BA           | 2162       | G           |
| 22         | BA           | 2163       | A           |
| 22         | BA           | 2164       | C           |
| 22         | BA           | 2165       | C           |
| 22         | BA           | 2166       | U           |
| 22         | BA           | 2167       | U           |
| 22         | BA           | 2169       | A           |
| 22         | BA           | 2170       | A           |
| 22         | BA           | 2171       | A           |
| 22         | BA           | 2172       | U           |
| 22         | BA           | 2173       | A           |
| 22         | BA           | 2176       | A           |
| 22         | BA           | 2178       | C           |
| 22         | BA           | 2179       | C           |
| 22         | BA           | 2181       | U           |
| 22         | BA           | 2182       | U           |
| 22         | BA           | 2187       | U           |
| 22         | BA           | 2188       | U           |
| 22         | BA           | 2190       | G           |
| 22         | BA           | 2197       | U           |
| 22         | BA           | 2198       | A           |
| 22         | BA           | 2203       | U           |
| 22         | BA           | 2204       | G           |
| 22         | BA           | 2210       | U           |
| 22         | BA           | 2211       | A           |
| 22         | BA           | 2212       | A           |
| 22         | BA           | 2214       | C           |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 22  | BA    | 2220 | U    |
| 22  | BA    | 2225 | A    |
| 22  | BA    | 2238 | G    |
| 22  | BA    | 2239 | G    |
| 22  | BA    | 2248 | C    |
| 22  | BA    | 2250 | G    |
| 22  | BA    | 2258 | C    |
| 22  | BA    | 2268 | A    |
| 22  | BA    | 2278 | A    |
| 22  | BA    | 2283 | C    |
| 22  | BA    | 2286 | G    |
| 22  | BA    | 2287 | A    |
| 22  | BA    | 2296 | U    |
| 22  | BA    | 2305 | U    |
| 22  | BA    | 2308 | G    |
| 22  | BA    | 2309 | A    |
| 22  | BA    | 2311 | A    |
| 22  | BA    | 2322 | A    |
| 22  | BA    | 2325 | G    |
| 22  | BA    | 2327 | A    |
| 22  | BA    | 2331 | G    |
| 22  | BA    | 2335 | A    |
| 22  | BA    | 2346 | A    |
| 22  | BA    | 2347 | C    |
| 22  | BA    | 2350 | C    |
| 22  | BA    | 2357 | G    |
| 22  | BA    | 2361 | G    |
| 22  | BA    | 2383 | G    |
| 22  | BA    | 2385 | C    |
| 22  | BA    | 2389 | G    |
| 22  | BA    | 2394 | C    |
| 22  | BA    | 2402 | U    |
| 22  | BA    | 2403 | C    |
| 22  | BA    | 2406 | A    |
| 22  | BA    | 2420 | C    |
| 22  | BA    | 2424 | C    |
| 22  | BA    | 2425 | A    |
| 22  | BA    | 2428 | G    |
| 22  | BA    | 2429 | G    |
| 22  | BA    | 2430 | A    |
| 22  | BA    | 2431 | U    |
| 22  | BA    | 2435 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 22  | BA    | 2441 | U    |
| 22  | BA    | 2446 | G    |
| 22  | BA    | 2448 | A    |
| 22  | BA    | 2456 | C    |
| 22  | BA    | 2465 | C    |
| 22  | BA    | 2469 | A    |
| 22  | BA    | 2474 | U    |
| 22  | BA    | 2476 | A    |
| 22  | BA    | 2487 | G    |
| 22  | BA    | 2490 | G    |
| 22  | BA    | 2491 | U    |
| 22  | BA    | 2497 | A    |
| 22  | BA    | 2498 | C    |
| 22  | BA    | 2502 | G    |
| 22  | BA    | 2504 | U    |
| 22  | BA    | 2505 | G    |
| 22  | BA    | 2506 | U    |
| 22  | BA    | 2507 | C    |
| 22  | BA    | 2515 | C    |
| 22  | BA    | 2518 | A    |
| 22  | BA    | 2529 | G    |
| 22  | BA    | 2535 | G    |
| 22  | BA    | 2554 | U    |
| 22  | BA    | 2555 | U    |
| 22  | BA    | 2556 | C    |
| 22  | BA    | 2566 | A    |
| 22  | BA    | 2567 | G    |
| 22  | BA    | 2573 | C    |
| 22  | BA    | 2578 | G    |
| 22  | BA    | 2594 | C    |
| 22  | BA    | 2602 | A    |
| 22  | BA    | 2603 | G    |
| 22  | BA    | 2609 | U    |
| 22  | BA    | 2613 | U    |
| 22  | BA    | 2629 | U    |
| 22  | BA    | 2630 | G    |
| 22  | BA    | 2662 | A    |
| 22  | BA    | 2663 | G    |
| 22  | BA    | 2689 | U    |
| 22  | BA    | 2690 | U    |
| 22  | BA    | 2714 | G    |
| 22  | BA    | 2726 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 22  | BA    | 2729 | G    |
| 22  | BA    | 2733 | A    |
| 22  | BA    | 2748 | A    |
| 22  | BA    | 2757 | A    |
| 22  | BA    | 2765 | A    |
| 22  | BA    | 2778 | A    |
| 22  | BA    | 2791 | G    |
| 22  | BA    | 2792 | A    |
| 22  | BA    | 2798 | U    |
| 22  | BA    | 2799 | A    |
| 22  | BA    | 2800 | A    |
| 22  | BA    | 2811 | G    |
| 22  | BA    | 2820 | A    |
| 22  | BA    | 2821 | A    |
| 22  | BA    | 2825 | G    |
| 22  | BA    | 2826 | A    |
| 22  | BA    | 2836 | U    |
| 22  | BA    | 2867 | G    |
| 22  | BA    | 2873 | A    |
| 22  | BA    | 2879 | A    |
| 22  | BA    | 2880 | C    |
| 22  | BA    | 2883 | A    |
| 22  | BA    | 2884 | U    |
| 22  | BA    | 2887 | A    |
| 22  | BA    | 2891 | U    |
| 22  | BA    | 2903 | U    |
| 23  | BB    | 2    | G    |
| 23  | BB    | 9    | G    |
| 23  | BB    | 15   | A    |
| 23  | BB    | 16   | G    |
| 23  | BB    | 25   | U    |
| 23  | BB    | 35   | C    |
| 23  | BB    | 37   | C    |
| 23  | BB    | 42   | C    |
| 23  | BB    | 44   | G    |
| 23  | BB    | 45   | A    |
| 23  | BB    | 56   | G    |
| 23  | BB    | 66   | A    |
| 23  | BB    | 89   | U    |
| 23  | BB    | 90   | C    |
| 23  | BB    | 91   | C    |
| 23  | BB    | 109  | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 23  | BB    | 119 | A    |
| 1   | CA    | 5   | U    |
| 1   | CA    | 6   | G    |
| 1   | CA    | 9   | G    |
| 1   | CA    | 17  | U    |
| 1   | CA    | 21  | G    |
| 1   | CA    | 32  | A    |
| 1   | CA    | 39  | G    |
| 1   | CA    | 47  | C    |
| 1   | CA    | 48  | C    |
| 1   | CA    | 51  | A    |
| 1   | CA    | 52  | C    |
| 1   | CA    | 67  | C    |
| 1   | CA    | 70  | U    |
| 1   | CA    | 71  | A    |
| 1   | CA    | 74  | A    |
| 1   | CA    | 75  | G    |
| 1   | CA    | 79  | G    |
| 1   | CA    | 80  | A    |
| 1   | CA    | 84  | U    |
| 1   | CA    | 85  | U    |
| 1   | CA    | 86  | G    |
| 1   | CA    | 87  | C    |
| 1   | CA    | 88  | U    |
| 1   | CA    | 91  | U    |
| 1   | CA    | 93  | U    |
| 1   | CA    | 94  | G    |
| 1   | CA    | 116 | A    |
| 1   | CA    | 117 | G    |
| 1   | CA    | 120 | A    |
| 1   | CA    | 121 | U    |
| 1   | CA    | 122 | G    |
| 1   | CA    | 130 | A    |
| 1   | CA    | 131 | A    |
| 1   | CA    | 135 | C    |
| 1   | CA    | 137 | U    |
| 1   | CA    | 142 | G    |
| 1   | CA    | 143 | A    |
| 1   | CA    | 144 | G    |
| 1   | CA    | 154 | U    |
| 1   | CA    | 155 | A    |
| 1   | CA    | 156 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | CA    | 159 | G    |
| 1   | CA    | 169 | C    |
| 1   | CA    | 173 | U    |
| 1   | CA    | 174 | A    |
| 1   | CA    | 181 | A    |
| 1   | CA    | 182 | A    |
| 1   | CA    | 183 | C    |
| 1   | CA    | 184 | G    |
| 1   | CA    | 191 | G    |
| 1   | CA    | 197 | A    |
| 1   | CA    | 200 | G    |
| 1   | CA    | 201 | G    |
| 1   | CA    | 204 | G    |
| 1   | CA    | 207 | C    |
| 1   | CA    | 208 | U    |
| 1   | CA    | 209 | U    |
| 1   | CA    | 210 | C    |
| 1   | CA    | 211 | G    |
| 1   | CA    | 212 | G    |
| 1   | CA    | 214 | C    |
| 1   | CA    | 240 | G    |
| 1   | CA    | 244 | U    |
| 1   | CA    | 245 | U    |
| 1   | CA    | 247 | G    |
| 1   | CA    | 250 | A    |
| 1   | CA    | 251 | G    |
| 1   | CA    | 253 | A    |
| 1   | CA    | 254 | G    |
| 1   | CA    | 266 | G    |
| 1   | CA    | 267 | C    |
| 1   | CA    | 269 | C    |
| 1   | CA    | 280 | C    |
| 1   | CA    | 289 | G    |
| 1   | CA    | 294 | U    |
| 1   | CA    | 316 | C    |
| 1   | CA    | 321 | A    |
| 1   | CA    | 328 | C    |
| 1   | CA    | 329 | A    |
| 1   | CA    | 330 | C    |
| 1   | CA    | 332 | G    |
| 1   | CA    | 345 | C    |
| 1   | CA    | 347 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | CA    | 352 | C    |
| 1   | CA    | 354 | G    |
| 1   | CA    | 367 | U    |
| 1   | CA    | 372 | C    |
| 1   | CA    | 376 | G    |
| 1   | CA    | 378 | G    |
| 1   | CA    | 384 | G    |
| 1   | CA    | 389 | A    |
| 1   | CA    | 390 | U    |
| 1   | CA    | 398 | U    |
| 1   | CA    | 399 | G    |
| 1   | CA    | 404 | G    |
| 1   | CA    | 406 | G    |
| 1   | CA    | 411 | A    |
| 1   | CA    | 412 | A    |
| 1   | CA    | 413 | G    |
| 1   | CA    | 421 | U    |
| 1   | CA    | 422 | C    |
| 1   | CA    | 424 | G    |
| 1   | CA    | 427 | U    |
| 1   | CA    | 429 | U    |
| 1   | CA    | 430 | A    |
| 1   | CA    | 439 | U    |
| 1   | CA    | 446 | G    |
| 1   | CA    | 457 | G    |
| 1   | CA    | 459 | A    |
| 1   | CA    | 463 | U    |
| 1   | CA    | 467 | U    |
| 1   | CA    | 468 | A    |
| 1   | CA    | 473 | U    |
| 1   | CA    | 474 | G    |
| 1   | CA    | 478 | A    |
| 1   | CA    | 479 | U    |
| 1   | CA    | 481 | G    |
| 1   | CA    | 484 | G    |
| 1   | CA    | 485 | U    |
| 1   | CA    | 486 | U    |
| 1   | CA    | 498 | A    |
| 1   | CA    | 500 | G    |
| 1   | CA    | 505 | G    |
| 1   | CA    | 509 | A    |
| 1   | CA    | 511 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | CA    | 518 | C    |
| 1   | CA    | 519 | C    |
| 1   | CA    | 527 | G    |
| 1   | CA    | 531 | U    |
| 1   | CA    | 532 | A    |
| 1   | CA    | 533 | A    |
| 1   | CA    | 545 | C    |
| 1   | CA    | 547 | A    |
| 1   | CA    | 550 | G    |
| 1   | CA    | 559 | A    |
| 1   | CA    | 564 | C    |
| 1   | CA    | 568 | G    |
| 1   | CA    | 570 | G    |
| 1   | CA    | 572 | A    |
| 1   | CA    | 573 | A    |
| 1   | CA    | 576 | C    |
| 1   | CA    | 581 | G    |
| 1   | CA    | 582 | C    |
| 1   | CA    | 615 | G    |
| 1   | CA    | 619 | U    |
| 1   | CA    | 622 | A    |
| 1   | CA    | 636 | U    |
| 1   | CA    | 650 | G    |
| 1   | CA    | 653 | U    |
| 1   | CA    | 654 | G    |
| 1   | CA    | 665 | A    |
| 1   | CA    | 687 | A    |
| 1   | CA    | 695 | A    |
| 1   | CA    | 702 | A    |
| 1   | CA    | 721 | G    |
| 1   | CA    | 723 | U    |
| 1   | CA    | 724 | G    |
| 1   | CA    | 731 | G    |
| 1   | CA    | 747 | A    |
| 1   | CA    | 755 | G    |
| 1   | CA    | 758 | C    |
| 1   | CA    | 765 | G    |
| 1   | CA    | 777 | A    |
| 1   | CA    | 785 | G    |
| 1   | CA    | 787 | A    |
| 1   | CA    | 793 | U    |
| 1   | CA    | 794 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | CA    | 799  | G    |
| 1   | CA    | 802  | A    |
| 1   | CA    | 812  | G    |
| 1   | CA    | 815  | A    |
| 1   | CA    | 817  | C    |
| 1   | CA    | 828  | U    |
| 1   | CA    | 832  | G    |
| 1   | CA    | 841  | C    |
| 1   | CA    | 842  | U    |
| 1   | CA    | 843  | U    |
| 1   | CA    | 844  | G    |
| 1   | CA    | 845  | A    |
| 1   | CA    | 846  | G    |
| 1   | CA    | 849  | G    |
| 1   | CA    | 874  | G    |
| 1   | CA    | 876  | C    |
| 1   | CA    | 880  | C    |
| 1   | CA    | 889  | A    |
| 1   | CA    | 906  | A    |
| 1   | CA    | 914  | A    |
| 1   | CA    | 919  | A    |
| 1   | CA    | 922  | G    |
| 1   | CA    | 926  | G    |
| 1   | CA    | 934  | C    |
| 1   | CA    | 935  | A    |
| 1   | CA    | 960  | U    |
| 1   | CA    | 964  | A    |
| 1   | CA    | 969  | A    |
| 1   | CA    | 971  | G    |
| 1   | CA    | 975  | A    |
| 1   | CA    | 976  | G    |
| 1   | CA    | 977  | A    |
| 1   | CA    | 983  | A    |
| 1   | CA    | 991  | U    |
| 1   | CA    | 992  | U    |
| 1   | CA    | 993  | G    |
| 1   | CA    | 994  | A    |
| 1   | CA    | 995  | C    |
| 1   | CA    | 996  | A    |
| 1   | CA    | 1004 | A    |
| 1   | CA    | 1008 | U    |
| 1   | CA    | 1018 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | CA    | 1020 | G    |
| 1   | CA    | 1025 | U    |
| 1   | CA    | 1026 | G    |
| 1   | CA    | 1027 | C    |
| 1   | CA    | 1028 | C    |
| 1   | CA    | 1030 | U    |
| 1   | CA    | 1031 | C    |
| 1   | CA    | 1032 | G    |
| 1   | CA    | 1033 | G    |
| 1   | CA    | 1034 | G    |
| 1   | CA    | 1037 | C    |
| 1   | CA    | 1039 | G    |
| 1   | CA    | 1042 | A    |
| 1   | CA    | 1043 | G    |
| 1   | CA    | 1044 | A    |
| 1   | CA    | 1047 | G    |
| 1   | CA    | 1050 | G    |
| 1   | CA    | 1052 | U    |
| 1   | CA    | 1054 | C    |
| 1   | CA    | 1055 | A    |
| 1   | CA    | 1065 | U    |
| 1   | CA    | 1069 | C    |
| 1   | CA    | 1070 | U    |
| 1   | CA    | 1072 | G    |
| 1   | CA    | 1073 | U    |
| 1   | CA    | 1086 | U    |
| 1   | CA    | 1094 | G    |
| 1   | CA    | 1095 | U    |
| 1   | CA    | 1101 | A    |
| 1   | CA    | 1104 | G    |
| 1   | CA    | 1124 | G    |
| 1   | CA    | 1125 | U    |
| 1   | CA    | 1129 | C    |
| 1   | CA    | 1133 | G    |
| 1   | CA    | 1134 | G    |
| 1   | CA    | 1136 | C    |
| 1   | CA    | 1137 | C    |
| 1   | CA    | 1139 | G    |
| 1   | CA    | 1140 | C    |
| 1   | CA    | 1141 | C    |
| 1   | CA    | 1142 | G    |
| 1   | CA    | 1145 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | CA    | 1154 | G    |
| 1   | CA    | 1157 | A    |
| 1   | CA    | 1159 | U    |
| 1   | CA    | 1160 | G    |
| 1   | CA    | 1161 | C    |
| 1   | CA    | 1168 | U    |
| 1   | CA    | 1181 | G    |
| 1   | CA    | 1182 | G    |
| 1   | CA    | 1184 | G    |
| 1   | CA    | 1196 | A    |
| 1   | CA    | 1198 | G    |
| 1   | CA    | 1202 | U    |
| 1   | CA    | 1212 | U    |
| 1   | CA    | 1213 | A    |
| 1   | CA    | 1222 | G    |
| 1   | CA    | 1227 | A    |
| 1   | CA    | 1228 | C    |
| 1   | CA    | 1230 | C    |
| 1   | CA    | 1236 | A    |
| 1   | CA    | 1238 | A    |
| 1   | CA    | 1239 | A    |
| 1   | CA    | 1240 | U    |
| 1   | CA    | 1253 | G    |
| 1   | CA    | 1257 | A    |
| 1   | CA    | 1259 | C    |
| 1   | CA    | 1260 | G    |
| 1   | CA    | 1275 | A    |
| 1   | CA    | 1280 | A    |
| 1   | CA    | 1285 | A    |
| 1   | CA    | 1286 | U    |
| 1   | CA    | 1287 | A    |
| 1   | CA    | 1297 | G    |
| 1   | CA    | 1299 | A    |
| 1   | CA    | 1301 | U    |
| 1   | CA    | 1305 | G    |
| 1   | CA    | 1312 | G    |
| 1   | CA    | 1317 | C    |
| 1   | CA    | 1318 | A    |
| 1   | CA    | 1320 | C    |
| 1   | CA    | 1322 | C    |
| 1   | CA    | 1323 | G    |
| 1   | CA    | 1324 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | CA    | 1332 | A    |
| 1   | CA    | 1336 | C    |
| 1   | CA    | 1337 | G    |
| 1   | CA    | 1338 | G    |
| 1   | CA    | 1346 | A    |
| 1   | CA    | 1353 | G    |
| 1   | CA    | 1362 | A    |
| 1   | CA    | 1363 | A    |
| 1   | CA    | 1368 | A    |
| 1   | CA    | 1379 | G    |
| 1   | CA    | 1381 | U    |
| 1   | CA    | 1382 | C    |
| 1   | CA    | 1418 | A    |
| 1   | CA    | 1441 | A    |
| 1   | CA    | 1442 | G    |
| 1   | CA    | 1446 | A    |
| 1   | CA    | 1451 | U    |
| 1   | CA    | 1452 | C    |
| 1   | CA    | 1454 | G    |
| 1   | CA    | 1475 | G    |
| 1   | CA    | 1477 | U    |
| 1   | CA    | 1491 | G    |
| 1   | CA    | 1492 | A    |
| 1   | CA    | 1497 | G    |
| 1   | CA    | 1503 | A    |
| 1   | CA    | 1505 | G    |
| 1   | CA    | 1506 | U    |
| 1   | CA    | 1507 | A    |
| 1   | CA    | 1509 | C    |
| 1   | CA    | 1517 | G    |
| 1   | CA    | 1519 | A    |
| 1   | CA    | 1529 | G    |
| 1   | CA    | 1530 | G    |
| 1   | CA    | 1533 | C    |
| 1   | CA    | 1534 | A    |
| 1   | CA    | 1535 | C    |
| 1   | CA    | 1536 | C    |
| 22  | DA    | 10   | A    |
| 22  | DA    | 15   | G    |
| 22  | DA    | 32   | C    |
| 22  | DA    | 34   | U    |
| 22  | DA    | 39   | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 22  | DA    | 42  | A    |
| 22  | DA    | 43  | G    |
| 22  | DA    | 46  | G    |
| 22  | DA    | 47  | C    |
| 22  | DA    | 55  | G    |
| 22  | DA    | 57  | C    |
| 22  | DA    | 61  | C    |
| 22  | DA    | 63  | A    |
| 22  | DA    | 64  | A    |
| 22  | DA    | 66  | C    |
| 22  | DA    | 70  | G    |
| 22  | DA    | 71  | A    |
| 22  | DA    | 73  | A    |
| 22  | DA    | 74  | A    |
| 22  | DA    | 75  | G    |
| 22  | DA    | 80  | G    |
| 22  | DA    | 81  | G    |
| 22  | DA    | 82  | U    |
| 22  | DA    | 83  | A    |
| 22  | DA    | 84  | A    |
| 22  | DA    | 85  | G    |
| 22  | DA    | 87  | U    |
| 22  | DA    | 91  | A    |
| 22  | DA    | 96  | C    |
| 22  | DA    | 97  | C    |
| 22  | DA    | 98  | G    |
| 22  | DA    | 101 | A    |
| 22  | DA    | 103 | A    |
| 22  | DA    | 104 | A    |
| 22  | DA    | 111 | A    |
| 22  | DA    | 118 | A    |
| 22  | DA    | 119 | A    |
| 22  | DA    | 120 | U    |
| 22  | DA    | 121 | G    |
| 22  | DA    | 128 | C    |
| 22  | DA    | 137 | U    |
| 22  | DA    | 138 | U    |
| 22  | DA    | 139 | U    |
| 22  | DA    | 140 | C    |
| 22  | DA    | 141 | G    |
| 22  | DA    | 142 | A    |
| 22  | DA    | 143 | C    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 22  | DA    | 145 | C    |
| 22  | DA    | 150 | U    |
| 22  | DA    | 155 | A    |
| 22  | DA    | 158 | U    |
| 22  | DA    | 159 | G    |
| 22  | DA    | 162 | U    |
| 22  | DA    | 166 | U    |
| 22  | DA    | 178 | G    |
| 22  | DA    | 180 | G    |
| 22  | DA    | 184 | C    |
| 22  | DA    | 185 | G    |
| 22  | DA    | 196 | A    |
| 22  | DA    | 199 | A    |
| 22  | DA    | 202 | U    |
| 22  | DA    | 206 | U    |
| 22  | DA    | 216 | A    |
| 22  | DA    | 221 | A    |
| 22  | DA    | 222 | A    |
| 22  | DA    | 223 | A    |
| 22  | DA    | 224 | U    |
| 22  | DA    | 225 | C    |
| 22  | DA    | 228 | C    |
| 22  | DA    | 233 | A    |
| 22  | DA    | 245 | G    |
| 22  | DA    | 248 | G    |
| 22  | DA    | 249 | C    |
| 22  | DA    | 251 | A    |
| 22  | DA    | 252 | G    |
| 22  | DA    | 258 | G    |
| 22  | DA    | 262 | A    |
| 22  | DA    | 265 | A    |
| 22  | DA    | 266 | G    |
| 22  | DA    | 271 | G    |
| 22  | DA    | 272 | A    |
| 22  | DA    | 276 | U    |
| 22  | DA    | 279 | A    |
| 22  | DA    | 281 | C    |
| 22  | DA    | 283 | G    |
| 22  | DA    | 285 | G    |
| 22  | DA    | 291 | G    |
| 22  | DA    | 294 | A    |
| 22  | DA    | 311 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 22  | DA    | 321 | U    |
| 22  | DA    | 329 | G    |
| 22  | DA    | 330 | A    |
| 22  | DA    | 335 | C    |
| 22  | DA    | 346 | A    |
| 22  | DA    | 348 | A    |
| 22  | DA    | 350 | G    |
| 22  | DA    | 361 | G    |
| 22  | DA    | 362 | A    |
| 22  | DA    | 367 | G    |
| 22  | DA    | 371 | A    |
| 22  | DA    | 372 | G    |
| 22  | DA    | 380 | G    |
| 22  | DA    | 385 | C    |
| 22  | DA    | 386 | G    |
| 22  | DA    | 387 | U    |
| 22  | DA    | 392 | U    |
| 22  | DA    | 396 | G    |
| 22  | DA    | 401 | A    |
| 22  | DA    | 405 | U    |
| 22  | DA    | 411 | G    |
| 22  | DA    | 412 | A    |
| 22  | DA    | 417 | C    |
| 22  | DA    | 420 | C    |
| 22  | DA    | 421 | C    |
| 22  | DA    | 424 | G    |
| 22  | DA    | 426 | C    |
| 22  | DA    | 430 | A    |
| 22  | DA    | 435 | C    |
| 22  | DA    | 444 | C    |
| 22  | DA    | 446 | G    |
| 22  | DA    | 448 | U    |
| 22  | DA    | 451 | U    |
| 22  | DA    | 455 | C    |
| 22  | DA    | 461 | C    |
| 22  | DA    | 462 | C    |
| 22  | DA    | 478 | A    |
| 22  | DA    | 480 | A    |
| 22  | DA    | 481 | G    |
| 22  | DA    | 490 | C    |
| 22  | DA    | 491 | G    |
| 22  | DA    | 496 | G    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 22  | DA    | 504 | A    |
| 22  | DA    | 505 | A    |
| 22  | DA    | 508 | A    |
| 22  | DA    | 509 | C    |
| 22  | DA    | 510 | C    |
| 22  | DA    | 511 | U    |
| 22  | DA    | 528 | A    |
| 22  | DA    | 531 | C    |
| 22  | DA    | 532 | A    |
| 22  | DA    | 533 | G    |
| 22  | DA    | 543 | G    |
| 22  | DA    | 544 | C    |
| 22  | DA    | 546 | U    |
| 22  | DA    | 547 | A    |
| 22  | DA    | 548 | G    |
| 22  | DA    | 549 | G    |
| 22  | DA    | 550 | C    |
| 22  | DA    | 563 | A    |
| 22  | DA    | 564 | C    |
| 22  | DA    | 568 | U    |
| 22  | DA    | 569 | U    |
| 22  | DA    | 572 | A    |
| 22  | DA    | 573 | U    |
| 22  | DA    | 575 | A    |
| 22  | DA    | 586 | A    |
| 22  | DA    | 588 | U    |
| 22  | DA    | 603 | A    |
| 22  | DA    | 613 | A    |
| 22  | DA    | 614 | A    |
| 22  | DA    | 615 | U    |
| 22  | DA    | 617 | G    |
| 22  | DA    | 627 | A    |
| 22  | DA    | 628 | G    |
| 22  | DA    | 631 | A    |
| 22  | DA    | 637 | A    |
| 22  | DA    | 642 | U    |
| 22  | DA    | 645 | C    |
| 22  | DA    | 647 | G    |
| 22  | DA    | 648 | G    |
| 22  | DA    | 649 | G    |
| 22  | DA    | 654 | A    |
| 22  | DA    | 655 | A    |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 22  | DA    | 656 | G    |
| 22  | DA    | 657 | U    |
| 22  | DA    | 664 | G    |
| 22  | DA    | 672 | C    |
| 22  | DA    | 682 | G    |
| 22  | DA    | 684 | G    |
| 22  | DA    | 685 | A    |
| 22  | DA    | 686 | U    |
| 22  | DA    | 694 | U    |
| 22  | DA    | 695 | G    |
| 22  | DA    | 696 | G    |
| 22  | DA    | 701 | G    |
| 22  | DA    | 702 | U    |
| 22  | DA    | 704 | G    |
| 22  | DA    | 717 | C    |
| 22  | DA    | 726 | G    |
| 22  | DA    | 727 | A    |
| 22  | DA    | 728 | G    |
| 22  | DA    | 729 | G    |
| 22  | DA    | 730 | A    |
| 22  | DA    | 740 | C    |
| 22  | DA    | 747 | U    |
| 22  | DA    | 748 | G    |
| 22  | DA    | 752 | A    |
| 22  | DA    | 757 | G    |
| 22  | DA    | 758 | C    |
| 22  | DA    | 771 | G    |
| 22  | DA    | 773 | U    |
| 22  | DA    | 775 | G    |
| 22  | DA    | 776 | G    |
| 22  | DA    | 777 | G    |
| 22  | DA    | 782 | A    |
| 22  | DA    | 784 | G    |
| 22  | DA    | 785 | G    |
| 22  | DA    | 790 | U    |
| 22  | DA    | 792 | A    |
| 22  | DA    | 793 | A    |
| 22  | DA    | 798 | G    |
| 22  | DA    | 800 | A    |
| 22  | DA    | 801 | G    |
| 22  | DA    | 802 | A    |
| 22  | DA    | 805 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 22  | DA    | 812  | C    |
| 22  | DA    | 814  | C    |
| 22  | DA    | 815  | C    |
| 22  | DA    | 819  | A    |
| 22  | DA    | 826  | U    |
| 22  | DA    | 827  | U    |
| 22  | DA    | 828  | U    |
| 22  | DA    | 829  | A    |
| 22  | DA    | 830  | G    |
| 22  | DA    | 844  | A    |
| 22  | DA    | 845  | A    |
| 22  | DA    | 846  | U    |
| 22  | DA    | 847  | U    |
| 22  | DA    | 858  | G    |
| 22  | DA    | 859  | G    |
| 22  | DA    | 878  | A    |
| 22  | DA    | 881  | G    |
| 22  | DA    | 882  | G    |
| 22  | DA    | 885  | C    |
| 22  | DA    | 896  | A    |
| 22  | DA    | 897  | C    |
| 22  | DA    | 907  | G    |
| 22  | DA    | 910  | A    |
| 22  | DA    | 914  | G    |
| 22  | DA    | 915  | C    |
| 22  | DA    | 931  | U    |
| 22  | DA    | 933  | A    |
| 22  | DA    | 941  | A    |
| 22  | DA    | 946  | C    |
| 22  | DA    | 953  | G    |
| 22  | DA    | 958  | U    |
| 22  | DA    | 959  | A    |
| 22  | DA    | 961  | C    |
| 22  | DA    | 974  | G    |
| 22  | DA    | 983  | A    |
| 22  | DA    | 995  | C    |
| 22  | DA    | 996  | A    |
| 22  | DA    | 1012 | U    |
| 22  | DA    | 1013 | C    |
| 22  | DA    | 1022 | G    |
| 22  | DA    | 1023 | U    |
| 22  | DA    | 1025 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 22  | DA    | 1026 | G    |
| 22  | DA    | 1033 | U    |
| 22  | DA    | 1046 | A    |
| 22  | DA    | 1047 | G    |
| 22  | DA    | 1057 | A    |
| 22  | DA    | 1058 | U    |
| 22  | DA    | 1061 | U    |
| 22  | DA    | 1062 | G    |
| 22  | DA    | 1065 | U    |
| 22  | DA    | 1066 | U    |
| 22  | DA    | 1067 | A    |
| 22  | DA    | 1068 | G    |
| 22  | DA    | 1069 | A    |
| 22  | DA    | 1070 | A    |
| 22  | DA    | 1071 | G    |
| 22  | DA    | 1072 | C    |
| 22  | DA    | 1075 | C    |
| 22  | DA    | 1077 | A    |
| 22  | DA    | 1088 | A    |
| 22  | DA    | 1089 | A    |
| 22  | DA    | 1092 | C    |
| 22  | DA    | 1094 | U    |
| 22  | DA    | 1096 | A    |
| 22  | DA    | 1097 | U    |
| 22  | DA    | 1098 | A    |
| 22  | DA    | 1100 | C    |
| 22  | DA    | 1101 | U    |
| 22  | DA    | 1104 | C    |
| 22  | DA    | 1110 | G    |
| 22  | DA    | 1112 | G    |
| 22  | DA    | 1115 | G    |
| 22  | DA    | 1116 | G    |
| 22  | DA    | 1119 | U    |
| 22  | DA    | 1128 | G    |
| 22  | DA    | 1132 | U    |
| 22  | DA    | 1135 | C    |
| 22  | DA    | 1136 | G    |
| 22  | DA    | 1139 | G    |
| 22  | DA    | 1153 | C    |
| 22  | DA    | 1155 | A    |
| 22  | DA    | 1171 | G    |
| 22  | DA    | 1172 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 22  | DA    | 1175 | A    |
| 22  | DA    | 1176 | U    |
| 22  | DA    | 1178 | C    |
| 22  | DA    | 1179 | G    |
| 22  | DA    | 1180 | U    |
| 22  | DA    | 1183 | U    |
| 22  | DA    | 1186 | G    |
| 22  | DA    | 1199 | U    |
| 22  | DA    | 1204 | A    |
| 22  | DA    | 1205 | A    |
| 22  | DA    | 1212 | G    |
| 22  | DA    | 1227 | G    |
| 22  | DA    | 1230 | A    |
| 22  | DA    | 1231 | U    |
| 22  | DA    | 1235 | G    |
| 22  | DA    | 1236 | G    |
| 22  | DA    | 1237 | A    |
| 22  | DA    | 1238 | G    |
| 22  | DA    | 1242 | U    |
| 22  | DA    | 1243 | C    |
| 22  | DA    | 1244 | A    |
| 22  | DA    | 1247 | A    |
| 22  | DA    | 1248 | G    |
| 22  | DA    | 1250 | G    |
| 22  | DA    | 1253 | A    |
| 22  | DA    | 1256 | G    |
| 22  | DA    | 1266 | G    |
| 22  | DA    | 1268 | A    |
| 22  | DA    | 1272 | A    |
| 22  | DA    | 1273 | U    |
| 22  | DA    | 1276 | A    |
| 22  | DA    | 1282 | U    |
| 22  | DA    | 1288 | G    |
| 22  | DA    | 1289 | C    |
| 22  | DA    | 1293 | C    |
| 22  | DA    | 1294 | U    |
| 22  | DA    | 1300 | G    |
| 22  | DA    | 1301 | A    |
| 22  | DA    | 1321 | A    |
| 22  | DA    | 1330 | C    |
| 22  | DA    | 1339 | G    |
| 22  | DA    | 1344 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 22  | DA    | 1345 | C    |
| 22  | DA    | 1352 | U    |
| 22  | DA    | 1355 | G    |
| 22  | DA    | 1359 | A    |
| 22  | DA    | 1365 | A    |
| 22  | DA    | 1374 | G    |
| 22  | DA    | 1376 | C    |
| 22  | DA    | 1378 | A    |
| 22  | DA    | 1379 | U    |
| 22  | DA    | 1380 | G    |
| 22  | DA    | 1383 | A    |
| 22  | DA    | 1384 | A    |
| 22  | DA    | 1391 | U    |
| 22  | DA    | 1393 | A    |
| 22  | DA    | 1395 | A    |
| 22  | DA    | 1411 | U    |
| 22  | DA    | 1416 | G    |
| 22  | DA    | 1418 | G    |
| 22  | DA    | 1419 | A    |
| 22  | DA    | 1420 | A    |
| 22  | DA    | 1428 | C    |
| 22  | DA    | 1434 | A    |
| 22  | DA    | 1446 | C    |
| 22  | DA    | 1452 | G    |
| 22  | DA    | 1456 | G    |
| 22  | DA    | 1458 | U    |
| 22  | DA    | 1462 | C    |
| 22  | DA    | 1465 | G    |
| 22  | DA    | 1468 | U    |
| 22  | DA    | 1471 | G    |
| 22  | DA    | 1476 | U    |
| 22  | DA    | 1482 | G    |
| 22  | DA    | 1493 | C    |
| 22  | DA    | 1503 | A    |
| 22  | DA    | 1504 | A    |
| 22  | DA    | 1509 | A    |
| 22  | DA    | 1510 | G    |
| 22  | DA    | 1515 | A    |
| 22  | DA    | 1523 | U    |
| 22  | DA    | 1524 | G    |
| 22  | DA    | 1527 | G    |
| 22  | DA    | 1530 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 22  | DA    | 1531 | C    |
| 22  | DA    | 1533 | C    |
| 22  | DA    | 1534 | U    |
| 22  | DA    | 1535 | A    |
| 22  | DA    | 1536 | C    |
| 22  | DA    | 1540 | G    |
| 22  | DA    | 1546 | G    |
| 22  | DA    | 1555 | G    |
| 22  | DA    | 1560 | G    |
| 22  | DA    | 1566 | A    |
| 22  | DA    | 1569 | A    |
| 22  | DA    | 1576 | U    |
| 22  | DA    | 1578 | U    |
| 22  | DA    | 1581 | G    |
| 22  | DA    | 1582 | C    |
| 22  | DA    | 1583 | A    |
| 22  | DA    | 1584 | U    |
| 22  | DA    | 1585 | C    |
| 22  | DA    | 1587 | G    |
| 22  | DA    | 1592 | C    |
| 22  | DA    | 1602 | U    |
| 22  | DA    | 1603 | A    |
| 22  | DA    | 1606 | C    |
| 22  | DA    | 1607 | C    |
| 22  | DA    | 1608 | A    |
| 22  | DA    | 1610 | A    |
| 22  | DA    | 1613 | G    |
| 22  | DA    | 1616 | A    |
| 22  | DA    | 1626 | A    |
| 22  | DA    | 1645 | G    |
| 22  | DA    | 1646 | C    |
| 22  | DA    | 1647 | U    |
| 22  | DA    | 1648 | U    |
| 22  | DA    | 1649 | G    |
| 22  | DA    | 1651 | G    |
| 22  | DA    | 1652 | A    |
| 22  | DA    | 1653 | G    |
| 22  | DA    | 1660 | G    |
| 22  | DA    | 1663 | G    |
| 22  | DA    | 1664 | A    |
| 22  | DA    | 1674 | G    |
| 22  | DA    | 1715 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 22  | DA    | 1729 | U    |
| 22  | DA    | 1730 | C    |
| 22  | DA    | 1732 | C    |
| 22  | DA    | 1738 | G    |
| 22  | DA    | 1740 | G    |
| 22  | DA    | 1744 | A    |
| 22  | DA    | 1750 | G    |
| 22  | DA    | 1758 | U    |
| 22  | DA    | 1764 | C    |
| 22  | DA    | 1773 | A    |
| 22  | DA    | 1781 | U    |
| 22  | DA    | 1791 | A    |
| 22  | DA    | 1793 | C    |
| 22  | DA    | 1800 | C    |
| 22  | DA    | 1802 | A    |
| 22  | DA    | 1808 | A    |
| 22  | DA    | 1810 | A    |
| 22  | DA    | 1812 | U    |
| 22  | DA    | 1816 | C    |
| 22  | DA    | 1817 | G    |
| 22  | DA    | 1829 | A    |
| 22  | DA    | 1848 | A    |
| 22  | DA    | 1858 | A    |
| 22  | DA    | 1870 | C    |
| 22  | DA    | 1871 | A    |
| 22  | DA    | 1872 | A    |
| 22  | DA    | 1873 | G    |
| 22  | DA    | 1876 | A    |
| 22  | DA    | 1878 | G    |
| 22  | DA    | 1880 | U    |
| 22  | DA    | 1882 | U    |
| 22  | DA    | 1889 | A    |
| 22  | DA    | 1903 | G    |
| 22  | DA    | 1906 | G    |
| 22  | DA    | 1914 | C    |
| 22  | DA    | 1920 | C    |
| 22  | DA    | 1926 | U    |
| 22  | DA    | 1927 | A    |
| 22  | DA    | 1929 | G    |
| 22  | DA    | 1930 | G    |
| 22  | DA    | 1937 | A    |
| 22  | DA    | 1938 | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 22  | DA    | 1945 | G    |
| 22  | DA    | 1955 | U    |
| 22  | DA    | 1965 | C    |
| 22  | DA    | 1967 | C    |
| 22  | DA    | 1970 | A    |
| 22  | DA    | 1971 | U    |
| 22  | DA    | 1972 | G    |
| 22  | DA    | 1975 | G    |
| 22  | DA    | 1981 | A    |
| 22  | DA    | 1991 | U    |
| 22  | DA    | 1992 | G    |
| 22  | DA    | 1993 | U    |
| 22  | DA    | 1997 | C    |
| 22  | DA    | 2004 | G    |
| 22  | DA    | 2007 | U    |
| 22  | DA    | 2018 | G    |
| 22  | DA    | 2020 | A    |
| 22  | DA    | 2021 | C    |
| 22  | DA    | 2022 | U    |
| 22  | DA    | 2023 | C    |
| 22  | DA    | 2030 | A    |
| 22  | DA    | 2031 | A    |
| 22  | DA    | 2033 | A    |
| 22  | DA    | 2043 | C    |
| 22  | DA    | 2049 | G    |
| 22  | DA    | 2051 | A    |
| 22  | DA    | 2055 | C    |
| 22  | DA    | 2056 | G    |
| 22  | DA    | 2060 | A    |
| 22  | DA    | 2061 | G    |
| 22  | DA    | 2062 | A    |
| 22  | DA    | 2064 | C    |
| 22  | DA    | 2069 | G    |
| 22  | DA    | 2075 | U    |
| 22  | DA    | 2080 | A    |
| 22  | DA    | 2087 | G    |
| 22  | DA    | 2092 | U    |
| 22  | DA    | 2093 | G    |
| 22  | DA    | 2108 | A    |
| 22  | DA    | 2110 | G    |
| 22  | DA    | 2111 | U    |
| 22  | DA    | 2112 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 22  | DA    | 2113 | U    |
| 22  | DA    | 2115 | G    |
| 22  | DA    | 2116 | G    |
| 22  | DA    | 2117 | A    |
| 22  | DA    | 2118 | U    |
| 22  | DA    | 2119 | A    |
| 22  | DA    | 2120 | G    |
| 22  | DA    | 2125 | G    |
| 22  | DA    | 2126 | A    |
| 22  | DA    | 2127 | G    |
| 22  | DA    | 2128 | G    |
| 22  | DA    | 2131 | U    |
| 22  | DA    | 2132 | U    |
| 22  | DA    | 2133 | G    |
| 22  | DA    | 2135 | A    |
| 22  | DA    | 2137 | U    |
| 22  | DA    | 2146 | C    |
| 22  | DA    | 2147 | A    |
| 22  | DA    | 2149 | U    |
| 22  | DA    | 2158 | A    |
| 22  | DA    | 2162 | G    |
| 22  | DA    | 2163 | A    |
| 22  | DA    | 2164 | C    |
| 22  | DA    | 2165 | C    |
| 22  | DA    | 2166 | U    |
| 22  | DA    | 2169 | A    |
| 22  | DA    | 2170 | A    |
| 22  | DA    | 2171 | A    |
| 22  | DA    | 2172 | U    |
| 22  | DA    | 2189 | U    |
| 22  | DA    | 2190 | G    |
| 22  | DA    | 2194 | U    |
| 22  | DA    | 2198 | A    |
| 22  | DA    | 2203 | U    |
| 22  | DA    | 2204 | G    |
| 22  | DA    | 2207 | C    |
| 22  | DA    | 2211 | A    |
| 22  | DA    | 2212 | A    |
| 22  | DA    | 2215 | C    |
| 22  | DA    | 2225 | A    |
| 22  | DA    | 2226 | C    |
| 22  | DA    | 2230 | G    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 22  | DA    | 2238 | G    |
| 22  | DA    | 2239 | G    |
| 22  | DA    | 2242 | G    |
| 22  | DA    | 2243 | U    |
| 22  | DA    | 2245 | U    |
| 22  | DA    | 2246 | G    |
| 22  | DA    | 2250 | G    |
| 22  | DA    | 2268 | A    |
| 22  | DA    | 2273 | A    |
| 22  | DA    | 2279 | G    |
| 22  | DA    | 2280 | G    |
| 22  | DA    | 2283 | C    |
| 22  | DA    | 2285 | C    |
| 22  | DA    | 2287 | A    |
| 22  | DA    | 2305 | U    |
| 22  | DA    | 2307 | G    |
| 22  | DA    | 2308 | G    |
| 22  | DA    | 2309 | A    |
| 22  | DA    | 2310 | C    |
| 22  | DA    | 2311 | A    |
| 22  | DA    | 2313 | C    |
| 22  | DA    | 2321 | U    |
| 22  | DA    | 2322 | A    |
| 22  | DA    | 2325 | G    |
| 22  | DA    | 2327 | A    |
| 22  | DA    | 2333 | A    |
| 22  | DA    | 2345 | G    |
| 22  | DA    | 2347 | C    |
| 22  | DA    | 2350 | C    |
| 22  | DA    | 2354 | C    |
| 22  | DA    | 2356 | U    |
| 22  | DA    | 2357 | G    |
| 22  | DA    | 2361 | G    |
| 22  | DA    | 2383 | G    |
| 22  | DA    | 2385 | C    |
| 22  | DA    | 2397 | G    |
| 22  | DA    | 2402 | U    |
| 22  | DA    | 2406 | A    |
| 22  | DA    | 2407 | A    |
| 22  | DA    | 2410 | G    |
| 22  | DA    | 2412 | A    |
| 22  | DA    | 2417 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 22  | DA    | 2423 | U    |
| 22  | DA    | 2424 | C    |
| 22  | DA    | 2425 | A    |
| 22  | DA    | 2426 | A    |
| 22  | DA    | 2429 | G    |
| 22  | DA    | 2430 | A    |
| 22  | DA    | 2431 | U    |
| 22  | DA    | 2435 | A    |
| 22  | DA    | 2436 | G    |
| 22  | DA    | 2441 | U    |
| 22  | DA    | 2447 | G    |
| 22  | DA    | 2448 | A    |
| 22  | DA    | 2449 | U    |
| 22  | DA    | 2476 | A    |
| 22  | DA    | 2484 | G    |
| 22  | DA    | 2491 | U    |
| 22  | DA    | 2502 | G    |
| 22  | DA    | 2503 | A    |
| 22  | DA    | 2505 | G    |
| 22  | DA    | 2517 | C    |
| 22  | DA    | 2518 | A    |
| 22  | DA    | 2525 | G    |
| 22  | DA    | 2529 | G    |
| 22  | DA    | 2535 | G    |
| 22  | DA    | 2547 | A    |
| 22  | DA    | 2550 | G    |
| 22  | DA    | 2554 | U    |
| 22  | DA    | 2556 | C    |
| 22  | DA    | 2563 | U    |
| 22  | DA    | 2566 | A    |
| 22  | DA    | 2567 | G    |
| 22  | DA    | 2573 | C    |
| 22  | DA    | 2578 | G    |
| 22  | DA    | 2585 | U    |
| 22  | DA    | 2586 | U    |
| 22  | DA    | 2600 | A    |
| 22  | DA    | 2602 | A    |
| 22  | DA    | 2603 | G    |
| 22  | DA    | 2609 | U    |
| 22  | DA    | 2613 | U    |
| 22  | DA    | 2615 | U    |
| 22  | DA    | 2619 | C    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 22  | DA    | 2629 | U    |
| 22  | DA    | 2630 | G    |
| 22  | DA    | 2644 | G    |
| 22  | DA    | 2646 | C    |
| 22  | DA    | 2648 | G    |
| 22  | DA    | 2656 | U    |
| 22  | DA    | 2661 | G    |
| 22  | DA    | 2663 | G    |
| 22  | DA    | 2665 | A    |
| 22  | DA    | 2682 | A    |
| 22  | DA    | 2688 | G    |
| 22  | DA    | 2689 | U    |
| 22  | DA    | 2690 | U    |
| 22  | DA    | 2691 | C    |
| 22  | DA    | 2714 | G    |
| 22  | DA    | 2716 | C    |
| 22  | DA    | 2718 | G    |
| 22  | DA    | 2726 | A    |
| 22  | DA    | 2727 | A    |
| 22  | DA    | 2729 | G    |
| 22  | DA    | 2739 | U    |
| 22  | DA    | 2748 | A    |
| 22  | DA    | 2751 | G    |
| 22  | DA    | 2757 | A    |
| 22  | DA    | 2778 | A    |
| 22  | DA    | 2791 | G    |
| 22  | DA    | 2794 | C    |
| 22  | DA    | 2799 | A    |
| 22  | DA    | 2803 | G    |
| 22  | DA    | 2809 | A    |
| 22  | DA    | 2812 | G    |
| 22  | DA    | 2820 | A    |
| 22  | DA    | 2823 | A    |
| 22  | DA    | 2825 | G    |
| 22  | DA    | 2826 | A    |
| 22  | DA    | 2833 | U    |
| 22  | DA    | 2834 | G    |
| 22  | DA    | 2835 | A    |
| 22  | DA    | 2843 | G    |
| 22  | DA    | 2850 | A    |
| 22  | DA    | 2852 | G    |
| 22  | DA    | 2861 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 22  | DA    | 2867 | G    |
| 22  | DA    | 2871 | U    |
| 22  | DA    | 2872 | A    |
| 22  | DA    | 2879 | A    |
| 22  | DA    | 2880 | C    |
| 22  | DA    | 2883 | A    |
| 22  | DA    | 2891 | U    |
| 22  | DA    | 2897 | U    |
| 23  | DB    | 13   | G    |
| 23  | DB    | 15   | A    |
| 23  | DB    | 16   | G    |
| 23  | DB    | 24   | G    |
| 23  | DB    | 35   | C    |
| 23  | DB    | 36   | C    |
| 23  | DB    | 44   | G    |
| 23  | DB    | 51   | G    |
| 23  | DB    | 54   | G    |
| 23  | DB    | 56   | G    |
| 23  | DB    | 61   | G    |
| 23  | DB    | 66   | A    |
| 23  | DB    | 87   | U    |
| 23  | DB    | 88   | C    |
| 23  | DB    | 89   | U    |
| 23  | DB    | 90   | C    |
| 23  | DB    | 99   | A    |
| 23  | DB    | 109  | A    |
| 23  | DB    | 110  | C    |
| 23  | DB    | 111  | U    |

All (75) RNA pucker outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | AA    | 209  | U    |
| 1   | AA    | 351  | G    |
| 1   | AA    | 429  | U    |
| 1   | AA    | 484  | G    |
| 1   | AA    | 722  | G    |
| 1   | AA    | 1031 | C    |
| 1   | AA    | 1049 | U    |
| 1   | AA    | 1145 | A    |
| 1   | AA    | 1201 | A    |
| 1   | AA    | 1211 | U    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 22  | BA    | 70   | G    |
| 22  | BA    | 199  | A    |
| 22  | BA    | 271  | G    |
| 22  | BA    | 310  | A    |
| 22  | BA    | 404  | A    |
| 22  | BA    | 668  | A    |
| 22  | BA    | 764  | A    |
| 22  | BA    | 784  | G    |
| 22  | BA    | 859  | G    |
| 22  | BA    | 892  | A    |
| 22  | BA    | 960  | A    |
| 22  | BA    | 984  | A    |
| 22  | BA    | 995  | C    |
| 22  | BA    | 1378 | A    |
| 22  | BA    | 1583 | A    |
| 22  | BA    | 1606 | C    |
| 22  | BA    | 1610 | A    |
| 22  | BA    | 1738 | G    |
| 22  | BA    | 1875 | G    |
| 22  | BA    | 1925 | C    |
| 22  | BA    | 2127 | G    |
| 22  | BA    | 2211 | A    |
| 22  | BA    | 2286 | G    |
| 22  | BA    | 2326 | C    |
| 22  | BA    | 2585 | U    |
| 22  | BA    | 2756 | U    |
| 22  | BA    | 2873 | A    |
| 1   | CA    | 85   | U    |
| 1   | CA    | 115  | G    |
| 1   | CA    | 209  | U    |
| 1   | CA    | 429  | U    |
| 1   | CA    | 484  | G    |
| 1   | CA    | 1049 | U    |
| 1   | CA    | 1201 | A    |
| 1   | CA    | 1211 | U    |
| 22  | DA    | 271  | G    |
| 22  | DA    | 404  | A    |
| 22  | DA    | 479  | A    |
| 22  | DA    | 613  | A    |
| 22  | DA    | 800  | A    |
| 22  | DA    | 846  | U    |
| 22  | DA    | 877  | A    |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 22  | DA    | 1237 | A    |
| 22  | DA    | 1275 | A    |
| 22  | DA    | 1344 | U    |
| 22  | DA    | 1378 | A    |
| 22  | DA    | 1475 | G    |
| 22  | DA    | 1514 | G    |
| 22  | DA    | 1606 | C    |
| 22  | DA    | 1847 | A    |
| 22  | DA    | 1875 | G    |
| 22  | DA    | 2109 | U    |
| 22  | DA    | 2127 | G    |
| 22  | DA    | 2145 | C    |
| 22  | DA    | 2146 | C    |
| 22  | DA    | 2162 | G    |
| 22  | DA    | 2211 | A    |
| 22  | DA    | 2225 | A    |
| 22  | DA    | 2286 | G    |
| 22  | DA    | 2307 | G    |
| 22  | DA    | 2308 | G    |
| 22  | DA    | 2326 | C    |
| 22  | DA    | 2425 | A    |
| 22  | DA    | 2655 | G    |
| 22  | DA    | 2756 | U    |

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 501 ligands modelled in this entry, 499 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res  | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |      |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 55  | DOL  | BA    | 3001 | -    | 43,50,50     | 2.84 | 15 (34%)    | 51,70,70    | 2.93 | 17 (33%)    |
| 55  | DOL  | DA    | 3001 | -    | 43,50,50     | 2.94 | 13 (30%)    | 51,70,70    | 2.84 | 11 (21%)    |

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

| Mol | Type | Chain | Res  | Link | Chirals | Torsions    | Rings   |
|-----|------|-------|------|------|---------|-------------|---------|
| 55  | DOL  | BA    | 3001 | -    | -       | 15/58/77/77 | 0/2/3/3 |
| 55  | DOL  | DA    | 3001 | -    | -       | 11/58/77/77 | 0/2/3/3 |

All (28) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 55  | DA    | 3001 | DOL  | O15-C14 | 9.24  | 1.37        | 1.21     |
| 55  | BA    | 3001 | DOL  | O15-C14 | 9.11  | 1.37        | 1.21     |
| 55  | DA    | 3001 | DOL  | C22-C23 | 7.99  | 1.52        | 1.32     |
| 55  | BA    | 3001 | DOL  | C22-C23 | 7.21  | 1.50        | 1.32     |
| 55  | BA    | 3001 | DOL  | O38-C37 | 6.58  | 1.37        | 1.21     |
| 55  | DA    | 3001 | DOL  | O38-C37 | 6.51  | 1.37        | 1.21     |
| 55  | DA    | 3001 | DOL  | C26-N25 | 6.15  | 1.47        | 1.34     |
| 55  | DA    | 3001 | DOL  | C19-C20 | 5.25  | 1.51        | 1.34     |
| 55  | BA    | 3001 | DOL  | C26-N25 | 5.10  | 1.45        | 1.34     |
| 55  | BA    | 3001 | DOL  | C19-C20 | 4.89  | 1.49        | 1.34     |
| 55  | DA    | 3001 | DOL  | C6-N5   | 4.57  | 1.45        | 1.34     |
| 55  | BA    | 3001 | DOL  | C6-N5   | 4.51  | 1.45        | 1.34     |
| 55  | BA    | 3001 | DOL  | C16-C17 | -3.73 | 1.48        | 1.54     |
| 55  | DA    | 3001 | DOL  | C28-C29 | 3.69  | 1.41        | 1.32     |
| 55  | BA    | 3001 | DOL  | O36-C32 | -3.54 | 1.39        | 1.44     |
| 55  | BA    | 3001 | DOL  | C28-C29 | 3.40  | 1.40        | 1.32     |
| 55  | DA    | 3001 | DOL  | O18-C17 | -3.34 | 1.37        | 1.43     |
| 55  | DA    | 3001 | DOL  | C16-C17 | -3.22 | 1.49        | 1.54     |
| 55  | DA    | 3001 | DOL  | C42-S39 | 3.12  | 1.83        | 1.78     |
| 55  | BA    | 3001 | DOL  | O18-C17 | -3.01 | 1.38        | 1.43     |
| 55  | BA    | 3001 | DOL  | O36-C37 | -2.96 | 1.27        | 1.34     |
| 55  | DA    | 3001 | DOL  | O36-C32 | -2.86 | 1.40        | 1.44     |
| 55  | DA    | 3001 | DOL  | C22-C20 | 2.85  | 1.52        | 1.45     |
| 55  | BA    | 3001 | DOL  | C3-C4   | 2.46  | 1.57        | 1.52     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 55  | DA    | 3001 | DOL  | O36-C37 | -2.29 | 1.29        | 1.34     |
| 55  | BA    | 3001 | DOL  | C1-N5   | -2.16 | 1.43        | 1.46     |
| 55  | BA    | 3001 | DOL  | C22-C20 | 2.13  | 1.50        | 1.45     |
| 55  | BA    | 3001 | DOL  | C42-S39 | 2.05  | 1.81        | 1.78     |

All (28) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 55  | DA    | 3001 | DOL  | O40-S39-O41 | -15.59 | 100.41      | 118.19   |
| 55  | BA    | 3001 | DOL  | O40-S39-O41 | -11.60 | 104.96      | 118.19   |
| 55  | BA    | 3001 | DOL  | C29-C28-C26 | -7.33  | 104.35      | 122.69   |
| 55  | BA    | 3001 | DOL  | C43-C42-S39 | 7.02   | 126.83      | 112.14   |
| 55  | BA    | 3001 | DOL  | C8-C6-N5    | 7.00   | 127.83      | 119.76   |
| 55  | DA    | 3001 | DOL  | C4-N5-C1    | -5.09  | 106.19      | 112.45   |
| 55  | BA    | 3001 | DOL  | C24-N25-C26 | -4.54  | 114.69      | 122.03   |
| 55  | DA    | 3001 | DOL  | C30-C29-C28 | -4.27  | 114.77      | 126.44   |
| 55  | DA    | 3001 | DOL  | C23-C22-C20 | -4.13  | 119.65      | 125.89   |
| 55  | BA    | 3001 | DOL  | O7-C6-N5    | -3.82  | 115.41      | 121.59   |
| 55  | BA    | 3001 | DOL  | C3-C2-C1    | 3.65   | 109.19      | 103.13   |
| 55  | DA    | 3001 | DOL  | C29-C28-C26 | -3.64  | 113.59      | 122.69   |
| 55  | BA    | 3001 | DOL  | C28-C26-N25 | 3.57   | 121.69      | 114.97   |
| 55  | DA    | 3001 | DOL  | C32-O36-C37 | 3.51   | 123.81      | 117.78   |
| 55  | DA    | 3001 | DOL  | C3-C2-C1    | 3.41   | 108.79      | 103.13   |
| 55  | DA    | 3001 | DOL  | O36-C37-C1  | 3.15   | 117.96      | 111.52   |
| 55  | BA    | 3001 | DOL  | C4-N5-C1    | -3.04  | 108.72      | 112.45   |
| 55  | BA    | 3001 | DOL  | O27-C26-N25 | -2.71  | 117.75      | 122.23   |
| 55  | BA    | 3001 | DOL  | C23-C22-C20 | -2.68  | 121.84      | 125.89   |
| 55  | BA    | 3001 | DOL  | O36-C37-C1  | 2.68   | 116.99      | 111.52   |
| 55  | BA    | 3001 | DOL  | C30-C29-C28 | -2.63  | 119.25      | 126.44   |
| 55  | DA    | 3001 | DOL  | C3-C4-N5    | -2.53  | 100.73      | 103.33   |
| 55  | BA    | 3001 | DOL  | C21-C20-C22 | 2.44   | 121.92      | 118.08   |
| 55  | DA    | 3001 | DOL  | C43-C42-S39 | 2.40   | 117.16      | 112.14   |
| 55  | BA    | 3001 | DOL  | O40-S39-C42 | 2.38   | 117.31      | 107.97   |
| 55  | DA    | 3001 | DOL  | C28-C26-N25 | 2.19   | 119.09      | 114.97   |
| 55  | BA    | 3001 | DOL  | C16-C17-C19 | -2.16  | 107.05      | 111.10   |
| 55  | BA    | 3001 | DOL  | O15-C14-C13 | -2.13  | 117.59      | 120.77   |

There are no chirality outliers.

All (26) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms          |
|-----|-------|------|------|----------------|
| 55  | BA    | 3001 | DOL  | C43-C42-S39-C2 |

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| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 55  | BA    | 3001 | DOL  | C43-C42-S39-O41 |
| 55  | BA    | 3001 | DOL  | C43-C42-S39-O40 |
| 55  | BA    | 3001 | DOL  | S39-C42-C43-N44 |
| 55  | BA    | 3001 | DOL  | N25-C26-C28-C29 |
| 55  | BA    | 3001 | DOL  | O27-C26-C28-C29 |
| 55  | DA    | 3001 | DOL  | N25-C26-C28-C29 |
| 55  | BA    | 3001 | DOL  | C21-C20-C22-C23 |
| 55  | BA    | 3001 | DOL  | C19-C20-C22-C23 |
| 55  | DA    | 3001 | DOL  | C28-C29-C30-C31 |
| 55  | DA    | 3001 | DOL  | O27-C26-C28-C29 |
| 55  | DA    | 3001 | DOL  | C46-C45-N44-C47 |
| 55  | BA    | 3001 | DOL  | C46-C45-N44-C43 |
| 55  | BA    | 3001 | DOL  | C46-C45-N44-C47 |
| 55  | DA    | 3001 | DOL  | C46-C45-N44-C43 |
| 55  | DA    | 3001 | DOL  | C2-C1-C37-O38   |
| 55  | DA    | 3001 | DOL  | C2-C1-C37-O36   |
| 55  | BA    | 3001 | DOL  | O36-C32-C33-C34 |
| 55  | DA    | 3001 | DOL  | C43-C42-S39-C2  |
| 55  | DA    | 3001 | DOL  | C10-C13-C14-C16 |
| 55  | DA    | 3001 | DOL  | C10-C13-C14-O15 |
| 55  | BA    | 3001 | DOL  | C28-C29-C30-C31 |
| 55  | BA    | 3001 | DOL  | C30-C32-C33-C35 |
| 55  | BA    | 3001 | DOL  | O36-C32-C33-C35 |
| 55  | BA    | 3001 | DOL  | C42-C43-N44-C45 |
| 55  | DA    | 3001 | DOL  | C42-C43-N44-C47 |

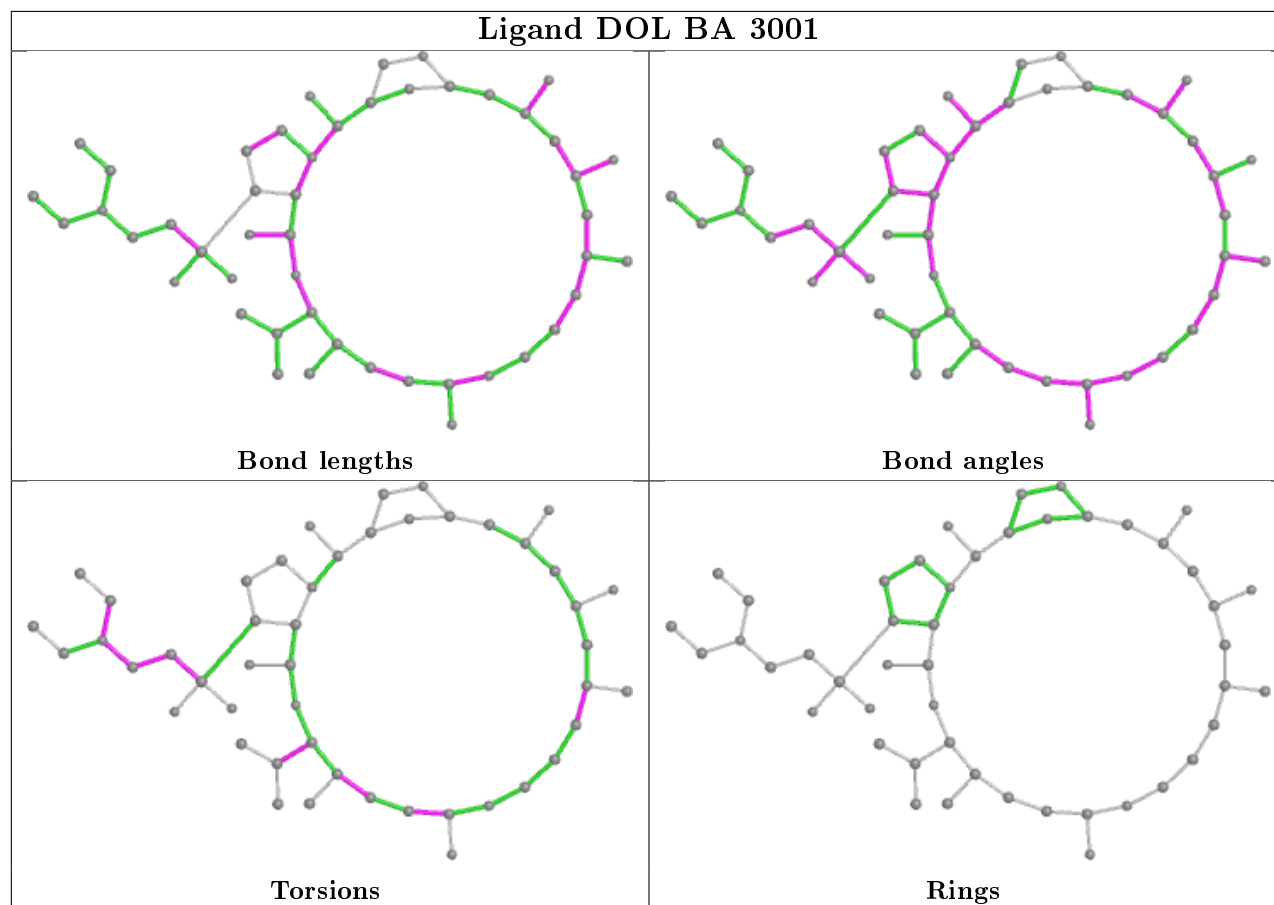
There are no ring outliers.

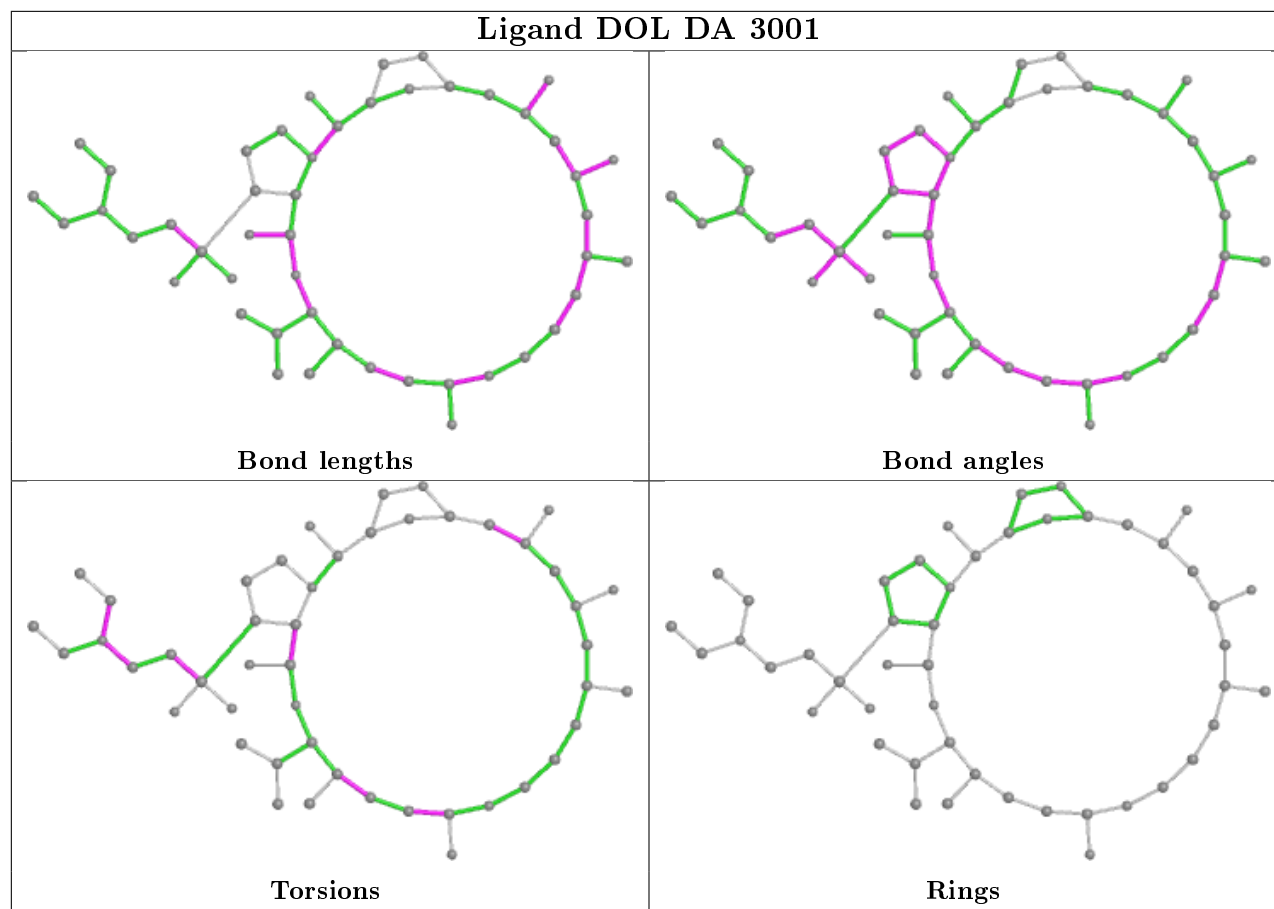
2 monomers are involved in 38 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 55  | BA    | 3001 | DOL  | 11      | 0            |
| 55  | DA    | 3001 | DOL  | 27      | 0            |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed         | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|------------------|--------|---------------|-----------------------|-------|
| 1   | AA    | 1538/1539 (99%)  | -0.11  | 34 (2%) 62 59 | 11, 51, 132, 183      | 0     |
| 1   | CA    | 1539/1539 (100%) | 0.35   | 125 (8%) 12 9 | 24, 70, 147, 178      | 0     |
| 2   | AB    | 218/218 (100%)   | 1.02   | 38 (17%) 1 1  | 40, 75, 101, 117      | 0     |
| 2   | CB    | 218/218 (100%)   | 1.08   | 47 (21%) 0 0  | 60, 88, 108, 123      | 0     |
| 3   | AC    | 206/206 (100%)   | 0.17   | 7 (3%) 45 40  | 37, 58, 80, 95        | 0     |
| 3   | CC    | 206/206 (100%)   | 0.98   | 35 (16%) 1 1  | 55, 80, 98, 108       | 0     |
| 4   | AD    | 205/205 (100%)   | 0.29   | 9 (4%) 34 30  | 33, 57, 80, 100       | 0     |
| 4   | CD    | 205/205 (100%)   | -0.08  | 6 (2%) 51 47  | 15, 36, 60, 84        | 0     |
| 5   | AE    | 150/150 (100%)   | 0.15   | 3 (2%) 65 63  | 29, 48, 78, 94        | 0     |
| 5   | CE    | 150/150 (100%)   | 0.27   | 7 (4%) 31 28  | 27, 53, 83, 104       | 0     |
| 6   | AF    | 100/100 (100%)   | 0.48   | 10 (10%) 7 5  | 35, 56, 75, 79        | 0     |
| 6   | CF    | 100/100 (100%)   | 0.54   | 6 (6%) 21 18  | 43, 73, 92, 104       | 0     |
| 7   | AG    | 151/151 (100%)   | 0.79   | 17 (11%) 5 4  | 54, 76, 92, 100       | 0     |
| 7   | CG    | 151/151 (100%)   | 2.73   | 88 (58%) 0 0  | 82, 106, 115, 119     | 0     |
| 8   | AH    | 129/129 (100%)   | 0.02   | 2 (1%) 72 71  | 29, 48, 68, 79        | 0     |
| 8   | CH    | 129/129 (100%)   | 0.26   | 4 (3%) 49 44  | 48, 64, 81, 96        | 0     |
| 9   | AI    | 127/127 (100%)   | 1.09   | 24 (18%) 1 0  | 45, 75, 98, 107       | 0     |
| 9   | CI    | 127/127 (100%)   | 1.74   | 44 (34%) 0 0  | 81, 97, 114, 121      | 0     |
| 10  | AJ    | 98/98 (100%)     | 0.82   | 16 (16%) 1 1  | 41, 68, 88, 116       | 0     |
| 10  | CJ    | 98/98 (100%)     | 2.56   | 53 (54%) 0 0  | 73, 98, 115, 124      | 0     |
| 11  | AK    | 117/117 (100%)   | 0.44   | 12 (10%) 6 5  | 28, 62, 92, 120       | 0     |
| 11  | CK    | 117/117 (100%)   | 0.33   | 4 (3%) 45 40  | 36, 68, 82, 90        | 0     |
| 12  | AL    | 123/123 (100%)   | 0.05   | 4 (3%) 46 41  | 20, 35, 65, 97        | 0     |
| 12  | CL    | 123/123 (100%)   | 0.33   | 7 (5%) 23 19  | 33, 50, 75, 96        | 0     |

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| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2   | OWAB(Å²) |     | Q<0.9             |   |
|-----|-------|-----------------|--------|-----------|----------|-----|-------------------|---|
| 13  | AM    | 114/114 (100%)  | 1.16   | 26 (22%)  | 0        | 0   | 49, 72, 93, 104   | 0 |
| 13  | CM    | 114/114 (100%)  | 3.75   | 90 (78%)  | 0        | 0   | 94, 115, 124, 126 | 0 |
| 14  | AN    | 96/100 (96%)    | 0.71   | 11 (11%)  | 4        | 3   | 41, 62, 96, 105   | 0 |
| 14  | CN    | 96/100 (96%)    | 2.36   | 51 (53%)  | 0        | 0   | 71, 97, 116, 123  | 0 |
| 15  | AO    | 88/88 (100%)    | 0.20   | 3 (3%)    | 45       | 40  | 31, 48, 65, 90    | 0 |
| 15  | CO    | 88/88 (100%)    | 0.38   | 6 (6%)    | 17       | 13  | 38, 65, 80, 103   | 0 |
| 16  | AP    | 82/82 (100%)    | 0.33   | 4 (4%)    | 29       | 26  | 35, 48, 84, 109   | 0 |
| 16  | CP    | 82/82 (100%)    | 0.63   | 7 (8%)    | 10       | 8   | 45, 62, 92, 113   | 0 |
| 17  | AQ    | 80/80 (100%)    | 0.45   | 4 (5%)    | 28       | 25  | 28, 49, 75, 110   | 0 |
| 17  | CQ    | 80/80 (100%)    | 1.22   | 18 (22%)  | 0        | 0   | 43, 79, 98, 100   | 0 |
| 18  | AR    | 55/55 (100%)    | 0.67   | 8 (14%)   | 2        | 1   | 42, 55, 78, 101   | 0 |
| 18  | CR    | 55/55 (100%)    | 0.48   | 7 (12%)   | 3        | 2   | 36, 55, 78, 109   | 0 |
| 19  | AS    | 79/79 (100%)    | 1.31   | 24 (30%)  | 0        | 0   | 56, 72, 89, 97    | 0 |
| 19  | CS    | 79/79 (100%)    | 3.39   | 57 (72%)  | 0        | 0   | 98, 115, 124, 129 | 0 |
| 20  | AT    | 85/85 (100%)    | 0.46   | 7 (8%)    | 11       | 9   | 36, 48, 70, 95    | 0 |
| 20  | CT    | 85/85 (100%)    | 1.54   | 25 (29%)  | 0        | 0   | 54, 78, 96, 101   | 0 |
| 21  | AU    | 51/51 (100%)    | 1.44   | 17 (33%)  | 0        | 0   | 44, 76, 97, 105   | 0 |
| 21  | CU    | 51/51 (100%)    | 0.65   | 4 (7%)    | 13       | 10  | 45, 71, 100, 103  | 0 |
| 22  | BA    | 2897/2903 (99%) | 0.06   | 140 (4%)  | 30       | 27  | 1, 14, 129, 195   | 0 |
| 22  | DA    | 2897/2903 (99%) | 0.60   | 229 (7%)  | 12       | 10  | 41, 85, 148, 181  | 0 |
| 23  | BB    | 119/119 (100%)  | -0.41  | 0         | 100      | 100 | 2, 23, 50, 80     | 0 |
| 23  | DB    | 118/119 (99%)   | 0.77   | 14 (11%)  | 4        | 3   | 69, 115, 134, 143 | 0 |
| 24  | BC    | 271/271 (100%)  | -0.33  | 2 (0%)    | 87       | 87  | 2, 20, 37, 55     | 0 |
| 24  | DC    | 271/271 (100%)  | 0.46   | 12 (4%)   | 34       | 30  | 47, 64, 77, 96    | 0 |
| 25  | BD    | 209/209 (100%)  | -0.44  | 0         | 100      | 100 | 0, 10, 36, 65     | 0 |
| 25  | DD    | 209/209 (100%)  | 0.75   | 31 (14%)  | 2        | 1   | 53, 72, 88, 96    | 0 |
| 26  | BE    | 201/201 (100%)  | -0.37  | 0         | 100      | 100 | 2, 24, 55, 88     | 0 |
| 26  | DE    | 201/201 (100%)  | 1.40   | 50 (24%)  | 0        | 0   | 53, 90, 107, 114  | 0 |
| 27  | BF    | 177/177 (100%)  | 0.22   | 14 (7%)   | 12       | 10  | 23, 44, 76, 90    | 0 |
| 27  | DF    | 177/177 (100%)  | 3.11   | 120 (67%) | 0        | 0   | 97, 114, 126, 131 | 0 |
| 28  | BG    | 176/176 (100%)  | -0.29  | 1 (0%)    | 89       | 89  | 16, 36, 57, 72    | 0 |

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| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|----------------|--------|---------------|-----------------------|-------|
| 28  | DG    | 176/176 (100%) | 2.16   | 86 (48%) 0 0  | 77, 96, 111, 121      | 0     |
| 29  | BH    | 149/149 (100%) | 2.72   | 74 (49%) 0 0  | 25, 102, 121, 129     | 0     |
| 29  | DH    | 149/149 (100%) | 1.28   | 36 (24%) 0 0  | 25, 92, 107, 115      | 0     |
| 30  | BI    | 141/141 (100%) | 3.80   | 96 (68%) 0 0  | 90, 117, 127, 134     | 0     |
| 30  | DI    | 141/141 (100%) | 5.64   | 131 (92%) 0 0 | 105, 126, 137, 143    | 0     |
| 31  | BJ    | 142/142 (100%) | -0.37  | 0 100 100     | 1, 6, 23, 36          | 0     |
| 31  | DJ    | 142/142 (100%) | 0.55   | 10 (7%) 16 12 | 52, 69, 83, 91        | 0     |
| 32  | BK    | 122/122 (100%) | -0.36  | 0 100 100     | 3, 12, 31, 62         | 0     |
| 32  | DK    | 122/122 (100%) | 0.53   | 8 (6%) 18 14  | 48, 66, 84, 96        | 0     |
| 33  | BL    | 143/143 (100%) | -0.32  | 0 100 100     | 1, 19, 43, 65         | 0     |
| 33  | DL    | 143/143 (100%) | 1.70   | 53 (37%) 0 0  | 46, 87, 99, 115       | 0     |
| 34  | BM    | 136/136 (100%) | -0.45  | 0 100 100     | 1, 10, 30, 83         | 0     |
| 34  | DM    | 136/136 (100%) | 0.62   | 15 (11%) 5 4  | 42, 71, 86, 100       | 0     |
| 35  | BN    | 120/120 (100%) | -0.42  | 0 100 100     | 3, 8, 18, 63          | 0     |
| 35  | DN    | 120/120 (100%) | 0.99   | 18 (15%) 2 1  | 59, 79, 94, 112       | 0     |
| 36  | BO    | 116/116 (100%) | -0.32  | 0 100 100     | 14, 26, 45, 55        | 0     |
| 36  | DO    | 116/116 (100%) | 2.11   | 59 (50%) 0 0  | 86, 100, 111, 118     | 0     |
| 37  | BP    | 114/114 (100%) | -0.36  | 2 (1%) 68 67  | 8, 17, 41, 72         | 0     |
| 37  | DP    | 114/114 (100%) | 0.98   | 19 (16%) 1 1  | 61, 75, 86, 95        | 0     |
| 38  | BQ    | 117/117 (100%) | -0.31  | 0 100 100     | 0, 3, 13, 34          | 0     |
| 38  | DQ    | 117/117 (100%) | 1.02   | 19 (16%) 1 1  | 57, 71, 80, 89        | 0     |
| 39  | BR    | 103/103 (100%) | -0.38  | 0 100 100     | 1, 13, 30, 58         | 0     |
| 39  | DR    | 103/103 (100%) | 1.52   | 32 (31%) 0 0  | 58, 81, 94, 104       | 0     |
| 40  | BS    | 110/110 (100%) | -0.42  | 0 100 100     | 2, 5, 24, 66          | 0     |
| 40  | DS    | 110/110 (100%) | 1.19   | 22 (20%) 1 0  | 62, 80, 95, 106       | 0     |
| 41  | BT    | 93/93 (100%)   | 0.07   | 3 (3%) 47 43  | 9, 26, 68, 100        | 0     |
| 41  | DT    | 93/93 (100%)   | 2.09   | 48 (51%) 0 0  | 73, 92, 106, 115      | 0     |
| 42  | BU    | 102/102 (100%) | 0.22   | 11 (10%) 5 4  | 12, 29, 63, 79        | 0     |
| 42  | DU    | 102/102 (100%) | 2.75   | 58 (56%) 0 0  | 78, 96, 110, 122      | 0     |
| 43  | BV    | 94/94 (100%)   | -0.38  | 0 100 100     | 5, 21, 43, 55         | 0     |
| 43  | DV    | 94/94 (100%)   | 1.16   | 22 (23%) 0 0  | 74, 88, 99, 106       | 0     |

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| Mol | Chain | Analysed          | <RSRZ> | #RSRZ>2        | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-------------------|--------|----------------|-----------------------|-------|
| 44  | BW    | 76/76 (100%)      | -0.35  | 1 (1%) 77 77   | 5, 12, 30, 57         | 0     |
| 44  | DW    | 75/76 (98%)       | 1.42   | 22 (29%) 0 0   | 58, 83, 92, 105       | 0     |
| 45  | BX    | 77/77 (100%)      | -0.32  | 0 100 100      | 8, 22, 51, 68         | 0     |
| 45  | DX    | 77/77 (100%)      | 1.02   | 16 (20%) 1 0   | 50, 72, 87, 92        | 0     |
| 46  | BY    | 63/63 (100%)      | 0.21   | 3 (4%) 30 27   | 24, 41, 73, 95        | 0     |
| 46  | DY    | 63/63 (100%)      | 2.05   | 34 (53%) 0 0   | 82, 99, 107, 110      | 0     |
| 47  | BZ    | 58/58 (100%)      | -0.32  | 0 100 100      | 2, 9, 29, 35          | 0     |
| 47  | DZ    | 58/58 (100%)      | 0.80   | 6 (10%) 6 5    | 60, 74, 85, 103       | 0     |
| 48  | B0    | 56/56 (100%)      | -0.49  | 0 100 100      | 1, 10, 35, 60         | 0     |
| 48  | D0    | 56/56 (100%)      | 1.41   | 15 (26%) 0 0   | 52, 83, 98, 105       | 0     |
| 49  | B1    | 50/50 (100%)      | -0.20  | 0 100 100      | 15, 27, 51, 58        | 0     |
| 49  | D1    | 50/50 (100%)      | 2.05   | 22 (44%) 0 0   | 74, 90, 95, 105       | 0     |
| 50  | B2    | 46/46 (100%)      | -0.34  | 1 (2%) 62 59   | 5, 9, 16, 79          | 0     |
| 50  | D2    | 46/46 (100%)      | 1.23   | 12 (26%) 0 0   | 58, 72, 87, 102       | 0     |
| 51  | B3    | 64/64 (100%)      | -0.40  | 0 100 100      | 4, 10, 20, 29         | 0     |
| 51  | D3    | 64/64 (100%)      | 1.42   | 17 (26%) 0 0   | 62, 75, 84, 95        | 0     |
| 52  | B4    | 38/38 (100%)      | -0.08  | 1 (2%) 56 52   | 8, 19, 34, 54         | 0     |
| 52  | D4    | 38/38 (100%)      | 2.51   | 20 (52%) 0 0   | 64, 79, 90, 100       | 0     |
| 53  | B5    | 191/228 (83%)     | 6.30   | 188 (98%) 0 0  | 100, 122, 133, 142    | 0     |
| All | All   | 20734/20794 (99%) | 0.62   | 2764 (13%) 3 2 | 0, 64, 125, 195       | 0     |

All (2764) RSRZ outliers are listed below:

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 53  | B5    | 218  | THR  | 28.0 |
| 53  | B5    | 140  | ASN  | 21.5 |
| 29  | BH    | 130  | VAL  | 18.3 |
| 30  | BI    | 53   | LEU  | 17.3 |
| 10  | AJ    | 102  | LEU  | 17.2 |
| 22  | BA    | 2100 | G    | 16.8 |
| 22  | BA    | 2184 | A    | 16.3 |
| 30  | BI    | 54   | PRO  | 15.4 |
| 30  | DI    | 68   | THR  | 15.4 |
| 53  | B5    | 217  | THR  | 15.0 |
| 30  | BI    | 79   | LEU  | 14.8 |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 53         | B5           | 97         | GLY         | 14.6        |
| 30         | BI           | 2          | ALA         | 14.3        |
| 30         | DI           | 2          | ALA         | 14.1        |
| 53         | B5           | 170        | GLY         | 14.0        |
| 53         | B5           | 162        | ILE         | 14.0        |
| 22         | BA           | 2101       | A           | 13.9        |
| 53         | B5           | 147        | GLY         | 13.5        |
| 22         | BA           | 2135       | A           | 13.3        |
| 22         | BA           | 2148       | G           | 13.1        |
| 53         | B5           | 96         | GLY         | 13.0        |
| 1          | CA           | 1536       | C           | 12.8        |
| 30         | DI           | 130        | GLU         | 12.6        |
| 30         | DI           | 80         | LEU         | 12.5        |
| 53         | B5           | 173        | HIS         | 12.5        |
| 22         | BA           | 2121       | G           | 12.5        |
| 53         | B5           | 107        | GLY         | 12.5        |
| 30         | DI           | 67         | PHE         | 12.4        |
| 30         | DI           | 78         | VAL         | 12.4        |
| 53         | B5           | 214        | TYR         | 12.3        |
| 53         | B5           | 143        | ALA         | 12.3        |
| 30         | BI           | 12         | GLN         | 12.1        |
| 22         | BA           | 2102       | G           | 12.0        |
| 30         | DI           | 54         | PRO         | 12.0        |
| 30         | BI           | 4          | LYS         | 11.9        |
| 22         | DA           | 1073       | A           | 11.8        |
| 22         | BA           | 2103       | C           | 11.8        |
| 53         | B5           | 111        | PHE         | 11.8        |
| 53         | B5           | 122        | GLY         | 11.7        |
| 22         | BA           | 2174       | C           | 11.5        |
| 22         | BA           | 2147       | A           | 11.5        |
| 53         | B5           | 131        | ILE         | 11.5        |
| 30         | DI           | 3          | LYS         | 11.5        |
| 22         | BA           | 2159       | G           | 11.3        |
| 30         | DI           | 133        | ALA         | 11.3        |
| 22         | BA           | 2112       | G           | 11.3        |
| 53         | B5           | 106        | ASP         | 11.1        |
| 10         | CJ           | 74         | VAL         | 11.1        |
| 22         | BA           | 2117       | A           | 11.0        |
| 30         | BI           | 3          | LYS         | 11.0        |
| 22         | BA           | 2145       | C           | 11.0        |
| 53         | B5           | 76         | LEU         | 11.0        |
| 7          | CG           | 62         | PHE         | 10.9        |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 1          | CA           | 1538       | C           | 10.9        |
| 30         | DI           | 53         | LEU         | 10.9        |
| 22         | BA           | 2177       | C           | 10.9        |
| 22         | BA           | 2136       | G           | 10.9        |
| 22         | BA           | 2140       | G           | 10.9        |
| 1          | CA           | 1539       | C           | 10.9        |
| 30         | DI           | 129        | ILE         | 10.8        |
| 53         | B5           | 55         | SER         | 10.8        |
| 28         | DG           | 33         | LEU         | 10.8        |
| 22         | BA           | 2185       | U           | 10.7        |
| 22         | BA           | 2183       | A           | 10.7        |
| 22         | BA           | 2132       | U           | 10.7        |
| 13         | CM           | 45         | ILE         | 10.6        |
| 30         | BI           | 11         | LEU         | 10.6        |
| 53         | B5           | 157        | ILE         | 10.6        |
| 20         | CT           | 4          | ILE         | 10.5        |
| 30         | BI           | 69         | PHE         | 10.4        |
| 22         | BA           | 2160       | C           | 10.4        |
| 22         | BA           | 2176       | A           | 10.4        |
| 27         | DF           | 76         | GLY         | 10.3        |
| 22         | BA           | 2158       | A           | 10.2        |
| 53         | B5           | 95         | VAL         | 10.2        |
| 53         | B5           | 66         | PRO         | 10.2        |
| 29         | BH           | 98         | ASP         | 10.2        |
| 30         | DI           | 76         | ALA         | 10.2        |
| 2          | AB           | 157        | LEU         | 10.2        |
| 30         | DI           | 85         | GLY         | 10.1        |
| 22         | BA           | 2161       | C           | 10.0        |
| 29         | BH           | 97         | ARG         | 10.0        |
| 29         | BH           | 102        | ALA         | 10.0        |
| 22         | BA           | 2182       | U           | 9.9         |
| 53         | B5           | 68         | GLY         | 9.9         |
| 53         | B5           | 141        | PRO         | 9.8         |
| 22         | BA           | 2178       | C           | 9.8         |
| 22         | DA           | 1067       | A           | 9.7         |
| 9          | CI           | 128        | SER         | 9.6         |
| 29         | BH           | 101        | ASP         | 9.6         |
| 30         | BI           | 114        | ALA         | 9.6         |
| 22         | BA           | 2139       | U           | 9.5         |
| 13         | CM           | 10         | PRO         | 9.5         |
| 53         | B5           | 223        | VAL         | 9.4         |
| 22         | BA           | 2144       | G           | 9.4         |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 30  | DI    | 139  | VAL  | 9.4  |
| 1   | CA    | 1535 | C    | 9.4  |
| 30  | DI    | 69   | PHE  | 9.3  |
| 53  | B5    | 134  | PRO  | 9.3  |
| 22  | BA    | 2120 | G    | 9.2  |
| 29  | DH    | 142  | VAL  | 9.2  |
| 22  | BA    | 2169 | A    | 9.2  |
| 30  | BI    | 87   | LYS  | 9.2  |
| 22  | BA    | 2149 | U    | 9.2  |
| 22  | BA    | 2123 | G    | 9.1  |
| 30  | DI    | 52   | GLY  | 9.1  |
| 29  | BH    | 96   | THR  | 9.0  |
| 22  | BA    | 2124 | G    | 9.0  |
| 22  | BA    | 2156 | G    | 9.0  |
| 27  | DF    | 39   | GLY  | 9.0  |
| 22  | BA    | 2130 | U    | 8.9  |
| 30  | DI    | 22   | PRO  | 8.9  |
| 53  | B5    | 148  | PHE  | 8.9  |
| 53  | B5    | 142  | LYS  | 8.9  |
| 13  | CM    | 23   | TYR  | 8.9  |
| 53  | B5    | 165  | ARG  | 8.9  |
| 29  | BH    | 72   | ILE  | 8.8  |
| 29  | DH    | 136  | SER  | 8.8  |
| 53  | B5    | 98   | GLU  | 8.8  |
| 30  | DI    | 6    | GLN  | 8.8  |
| 30  | BI    | 80   | LEU  | 8.7  |
| 22  | BA    | 2104 | C    | 8.7  |
| 30  | DI    | 98   | VAL  | 8.7  |
| 22  | BA    | 2099 | U    | 8.7  |
| 30  | DI    | 120  | ALA  | 8.7  |
| 30  | DI    | 77   | ALA  | 8.6  |
| 30  | DI    | 56   | PRO  | 8.6  |
| 30  | DI    | 4    | LYS  | 8.5  |
| 30  | DI    | 110  | ALA  | 8.5  |
| 22  | BA    | 2111 | U    | 8.5  |
| 22  | BA    | 2138 | G    | 8.5  |
| 13  | CM    | 39   | ILE  | 8.5  |
| 28  | DG    | 32   | GLU  | 8.4  |
| 22  | BA    | 2143 | C    | 8.4  |
| 30  | DI    | 121  | ASP  | 8.4  |
| 53  | B5    | 62   | THR  | 8.4  |
| 53  | B5    | 87   | ALA  | 8.4  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 30  | BI    | 133  | ALA  | 8.4  |
| 2   | AB    | 156  | GLY  | 8.4  |
| 22  | BA    | 2162 | G    | 8.3  |
| 53  | B5    | 27   | ALA  | 8.3  |
| 1   | CA    | 1537 | U    | 8.3  |
| 13  | CM    | 63   | PHE  | 8.3  |
| 22  | DA    | 2174 | C    | 8.2  |
| 30  | DI    | 79   | LEU  | 8.2  |
| 22  | DA    | 1065 | U    | 8.2  |
| 14  | CN    | 20   | TYR  | 8.2  |
| 30  | DI    | 58   | VAL  | 8.2  |
| 22  | BA    | 2155 | U    | 8.2  |
| 53  | B5    | 84   | ILE  | 8.2  |
| 19  | CS    | 71   | LEU  | 8.2  |
| 22  | BA    | 2113 | U    | 8.2  |
| 53  | B5    | 219  | MET  | 8.2  |
| 53  | B5    | 183  | PRO  | 8.2  |
| 30  | DI    | 99   | GLY  | 8.2  |
| 7   | CG    | 111  | ARG  | 8.2  |
| 7   | CG    | 66   | LEU  | 8.1  |
| 53  | B5    | 109  | MET  | 8.1  |
| 53  | B5    | 207  | GLY  | 8.1  |
| 30  | BI    | 13   | VAL  | 8.1  |
| 30  | DI    | 82   | LYS  | 8.1  |
| 30  | DI    | 8    | TYR  | 8.1  |
| 36  | DO    | 65   | THR  | 8.1  |
| 53  | B5    | 155  | ARG  | 8.1  |
| 22  | BA    | 2180 | U    | 8.0  |
| 30  | BI    | 67   | PHE  | 8.0  |
| 30  | DI    | 28   | LEU  | 8.0  |
| 42  | DU    | 58   | ILE  | 8.0  |
| 53  | B5    | 174  | ALA  | 8.0  |
| 53  | B5    | 166  | ASN  | 8.0  |
| 30  | DI    | 60   | THR  | 8.0  |
| 53  | B5    | 45   | HIS  | 8.0  |
| 22  | BA    | 2118 | U    | 8.0  |
| 30  | DI    | 57   | VAL  | 7.9  |
| 30  | DI    | 23   | PRO  | 7.9  |
| 53  | B5    | 108  | TRP  | 7.9  |
| 22  | DA    | 2124 | G    | 7.9  |
| 53  | B5    | 94   | TYR  | 7.9  |
| 53  | B5    | 156  | GLU  | 7.9  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 22  | BA    | 2168 | G    | 7.9  |
| 27  | DF    | 128  | TYR  | 7.9  |
| 22  | BA    | 2166 | U    | 7.9  |
| 53  | B5    | 67   | HIS  | 7.9  |
| 36  | DO    | 64   | TYR  | 7.8  |
| 53  | B5    | 77   | ALA  | 7.9  |
| 30  | DI    | 25   | GLY  | 7.8  |
| 33  | DL    | 92   | LEU  | 7.8  |
| 29  | BH    | 146  | VAL  | 7.8  |
| 30  | DI    | 48   | SER  | 7.8  |
| 22  | BA    | 2115 | G    | 7.8  |
| 22  | BA    | 2107 | G    | 7.8  |
| 53  | B5    | 179  | ALA  | 7.8  |
| 1   | AA    | 86   | G    | 7.8  |
| 22  | BA    | 2172 | U    | 7.8  |
| 1   | CA    | 1020 | G    | 7.8  |
| 22  | DA    | 1537 | G    | 7.7  |
| 22  | BA    | 2142 | A    | 7.7  |
| 1   | AA    | 1536 | C    | 7.7  |
| 22  | DA    | 2309 | A    | 7.7  |
| 53  | B5    | 216  | THR  | 7.7  |
| 53  | B5    | 48   | LEU  | 7.7  |
| 26  | DE    | 119  | ILE  | 7.7  |
| 53  | B5    | 93   | ASP  | 7.7  |
| 30  | DI    | 59   | ILE  | 7.7  |
| 53  | B5    | 132  | LEU  | 7.7  |
| 9   | CI    | 130  | ARG  | 7.7  |
| 22  | DA    | 1175 | A    | 7.6  |
| 29  | BH    | 110  | VAL  | 7.6  |
| 19  | CS    | 67   | VAL  | 7.6  |
| 22  | BA    | 2116 | G    | 7.6  |
| 22  | BA    | 2152 | G    | 7.6  |
| 30  | DI    | 66   | SER  | 7.6  |
| 10  | CJ    | 77   | VAL  | 7.5  |
| 27  | DF    | 129  | SER  | 7.5  |
| 29  | BH    | 136  | SER  | 7.5  |
| 30  | DI    | 96   | ASP  | 7.5  |
| 13  | CM    | 95   | LEU  | 7.5  |
| 22  | BA    | 2179 | C    | 7.5  |
| 53  | B5    | 182  | PRO  | 7.5  |
| 27  | DF    | 147  | ASP  | 7.5  |
| 22  | BA    | 2157 | G    | 7.4  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 36  | DO    | 66   | GLY  | 7.4  |
| 42  | DU    | 89   | ASP  | 7.4  |
| 42  | DU    | 20   | GLY  | 7.4  |
| 1   | AA    | 1535 | C    | 7.4  |
| 30  | DI    | 90   | SER  | 7.3  |
| 13  | CM    | 84   | GLY  | 7.3  |
| 29  | BH    | 106  | ALA  | 7.3  |
| 53  | B5    | 180  | SER  | 7.3  |
| 22  | BA    | 2153 | C    | 7.3  |
| 22  | BA    | 2165 | C    | 7.3  |
| 27  | DF    | 35   | THR  | 7.3  |
| 1   | AA    | 78   | A    | 7.2  |
| 1   | CA    | 1032 | G    | 7.2  |
| 19  | CS    | 80   | TYR  | 7.2  |
| 53  | B5    | 78   | ILE  | 7.2  |
| 2   | CB    | 32   | PHE  | 7.2  |
| 53  | B5    | 81   | GLY  | 7.2  |
| 4   | AD    | 37   | ALA  | 7.2  |
| 52  | D4    | 10   | LEU  | 7.2  |
| 53  | B5    | 59   | VAL  | 7.2  |
| 30  | BI    | 115  | ALA  | 7.2  |
| 28  | DG    | 62   | TRP  | 7.2  |
| 22  | BA    | 2163 | A    | 7.2  |
| 53  | B5    | 154  | ILE  | 7.1  |
| 19  | CS    | 60   | VAL  | 7.1  |
| 53  | B5    | 20   | VAL  | 7.1  |
| 1   | AA    | 1538 | C    | 7.1  |
| 14  | CN    | 36   | ALA  | 7.1  |
| 53  | B5    | 208  | THR  | 7.1  |
| 42  | DU    | 52   | LEU  | 7.1  |
| 30  | BI    | 5    | VAL  | 7.1  |
| 30  | DI    | 95   | LYS  | 7.1  |
| 53  | B5    | 161  | ARG  | 7.1  |
| 22  | BA    | 2181 | U    | 7.1  |
| 22  | DA    | 1093 | G    | 7.1  |
| 1   | AA    | 1539 | C    | 7.1  |
| 42  | DU    | 51   | ALA  | 7.1  |
| 53  | B5    | 46   | ALA  | 7.1  |
| 14  | CN    | 51   | LEU  | 7.0  |
| 1   | CA    | 1024 | G    | 7.0  |
| 53  | B5    | 85   | LYS  | 7.0  |
| 30  | BI    | 88   | SER  | 7.0  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 14  | CN    | 4    | GLN  | 7.0  |
| 1   | CA    | 1022 | A    | 7.0  |
| 53  | B5    | 104  | ILE  | 7.0  |
| 13  | CM    | 85   | CYS  | 7.0  |
| 53  | B5    | 42   | VAL  | 7.0  |
| 22  | BA    | 2114 | A    | 7.0  |
| 53  | B5    | 100  | ILE  | 7.0  |
| 42  | DU    | 78   | GLY  | 7.0  |
| 53  | B5    | 69   | LEU  | 6.9  |
| 53  | B5    | 146  | VAL  | 6.9  |
| 10  | CJ    | 76   | ILE  | 6.9  |
| 7   | AG    | 5    | ARG  | 6.9  |
| 42  | DU    | 50   | PRO  | 6.9  |
| 22  | BA    | 2175 | C    | 6.9  |
| 29  | BH    | 69   | ALA  | 6.8  |
| 53  | B5    | 171  | ALA  | 6.8  |
| 30  | DI    | 61   | VAL  | 6.8  |
| 38  | DQ    | 29   | SER  | 6.8  |
| 29  | BH    | 68   | ARG  | 6.8  |
| 28  | DG    | 105  | LEU  | 6.8  |
| 4   | CD    | 25   | VAL  | 6.8  |
| 19  | CS    | 74   | PHE  | 6.8  |
| 27  | DF    | 79   | ILE  | 6.8  |
| 2   | AB    | 136  | MET  | 6.7  |
| 22  | BA    | 2122 | U    | 6.7  |
| 22  | BA    | 2127 | G    | 6.7  |
| 30  | DI    | 55   | ILE  | 6.7  |
| 9   | AI    | 43   | THR  | 6.7  |
| 22  | BA    | 2134 | A    | 6.7  |
| 22  | BA    | 2154 | A    | 6.7  |
| 1   | CA    | 1030 | U    | 6.7  |
| 9   | AI    | 130  | ARG  | 6.7  |
| 27  | DF    | 113  | ASP  | 6.7  |
| 13  | CM    | 22   | ILE  | 6.7  |
| 22  | BA    | 2141 | G    | 6.7  |
| 7   | CG    | 88   | PRO  | 6.7  |
| 7   | CG    | 41   | SER  | 6.7  |
| 52  | D4    | 25   | VAL  | 6.6  |
| 13  | CM    | 69   | LEU  | 6.6  |
| 19  | CS    | 24   | GLU  | 6.6  |
| 22  | BA    | 2164 | C    | 6.6  |
| 7   | CG    | 133  | THR  | 6.6  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 27  | DF    | 24   | SER  | 6.6  |
| 12  | AL    | 124  | ALA  | 6.6  |
| 7   | CG    | 52   | GLN  | 6.6  |
| 22  | DA    | 1057 | A    | 6.6  |
| 42  | DU    | 39   | ILE  | 6.6  |
| 53  | B5    | 213  | VAL  | 6.6  |
| 30  | DI    | 73   | THR  | 6.5  |
| 30  | DI    | 5    | VAL  | 6.5  |
| 29  | BH    | 105  | ALA  | 6.5  |
| 1   | CA    | 1534 | A    | 6.5  |
| 30  | BI    | 99   | GLY  | 6.5  |
| 13  | CM    | 83   | LEU  | 6.5  |
| 27  | DF    | 112  | ARG  | 6.5  |
| 42  | DU    | 12   | ILE  | 6.5  |
| 22  | BA    | 2110 | G    | 6.5  |
| 30  | DI    | 46   | THR  | 6.5  |
| 19  | CS    | 51   | VAL  | 6.4  |
| 22  | BA    | 2150 | C    | 6.4  |
| 53  | B5    | 160  | GLY  | 6.4  |
| 13  | CM    | 64   | VAL  | 6.4  |
| 22  | DA    | 1077 | A    | 6.4  |
| 53  | B5    | 86   | GLU  | 6.4  |
| 44  | DW    | 52   | GLY  | 6.4  |
| 7   | CG    | 151  | PHE  | 6.4  |
| 22  | DA    | 1536 | C    | 6.4  |
| 2   | CB    | 135  | LEU  | 6.4  |
| 29  | BH    | 54   | LEU  | 6.4  |
| 14  | CN    | 52   | PRO  | 6.4  |
| 30  | DI    | 34   | ASN  | 6.3  |
| 53  | B5    | 64   | SER  | 6.3  |
| 53  | B5    | 37   | LYS  | 6.3  |
| 53  | B5    | 72   | GLN  | 6.3  |
| 53  | B5    | 80   | LYS  | 6.3  |
| 27  | DF    | 78   | LYS  | 6.3  |
| 29  | BH    | 85   | GLY  | 6.3  |
| 42  | DU    | 87   | PHE  | 6.3  |
| 27  | DF    | 43   | ALA  | 6.3  |
| 53  | B5    | 70   | GLY  | 6.3  |
| 1   | AA    | 1030 | U    | 6.3  |
| 30  | DI    | 75   | PRO  | 6.3  |
| 30  | DI    | 83   | ALA  | 6.3  |
| 19  | CS    | 31   | LEU  | 6.3  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 27  | DF    | 28   | VAL  | 6.3  |
| 37  | DP    | 115  | ASN  | 6.3  |
| 30  | DI    | 11   | LEU  | 6.3  |
| 53  | B5    | 151  | GLY  | 6.3  |
| 9   | AI    | 129  | LYS  | 6.2  |
| 22  | DA    | 2169 | A    | 6.2  |
| 53  | B5    | 110  | ASP  | 6.2  |
| 27  | DF    | 114  | PHE  | 6.2  |
| 53  | B5    | 199  | ALA  | 6.2  |
| 53  | B5    | 224  | ARG  | 6.2  |
| 1   | CA    | 1016 | A    | 6.2  |
| 7   | CG    | 57   | SER  | 6.2  |
| 22  | DA    | 2126 | A    | 6.2  |
| 27  | DF    | 21   | ASN  | 6.2  |
| 30  | BI    | 22   | PRO  | 6.2  |
| 30  | DI    | 47   | ASP  | 6.2  |
| 1   | CA    | 1025 | U    | 6.2  |
| 19  | CS    | 29   | LYS  | 6.2  |
| 9   | CI    | 43   | THR  | 6.2  |
| 27  | DF    | 130  | MET  | 6.2  |
| 1   | CA    | 1302 | C    | 6.1  |
| 53  | B5    | 158  | LYS  | 6.1  |
| 53  | B5    | 52   | PRO  | 6.1  |
| 7   | CG    | 54   | SER  | 6.1  |
| 13  | CM    | 32   | ALA  | 6.1  |
| 30  | BI    | 101  | ILE  | 6.1  |
| 30  | DI    | 118  | THR  | 6.1  |
| 53  | B5    | 149  | ASN  | 6.1  |
| 1   | CA    | 1031 | C    | 6.1  |
| 30  | DI    | 140  | VAL  | 6.1  |
| 30  | DI    | 114  | ALA  | 6.1  |
| 41  | DT    | 2    | ILE  | 6.1  |
| 45  | DX    | 49   | LEU  | 6.1  |
| 30  | BI    | 25   | GLY  | 6.1  |
| 7   | CG    | 118  | LEU  | 6.1  |
| 22  | BA    | 2167 | U    | 6.1  |
| 53  | B5    | 194  | ILE  | 6.1  |
| 19  | CS    | 30   | PRO  | 6.1  |
| 20  | CT    | 38   | ALA  | 6.1  |
| 53  | B5    | 105  | LEU  | 6.0  |
| 22  | BA    | 2171 | A    | 6.0  |
| 28  | DG    | 166  | ASP  | 6.0  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 53  | B5    | 26   | ALA  | 6.0  |
| 30  | DI    | 131  | GLY  | 6.0  |
| 30  | DI    | 142  | ASP  | 6.0  |
| 42  | DU    | 60   | GLU  | 6.0  |
| 30  | BI    | 100  | LYS  | 6.0  |
| 1   | CA    | 1018 | G    | 6.0  |
| 30  | BI    | 97   | LYS  | 6.0  |
| 53  | B5    | 198  | GLU  | 6.0  |
| 19  | CS    | 72   | GLY  | 6.0  |
| 42  | DU    | 35   | ILE  | 6.0  |
| 22  | BA    | 2126 | A    | 6.0  |
| 22  | DA    | 1078 | U    | 6.0  |
| 29  | BH    | 119  | ASN  | 6.0  |
| 30  | DI    | 21   | SER  | 5.9  |
| 19  | CS    | 66   | MET  | 5.9  |
| 29  | BH    | 121  | VAL  | 5.9  |
| 29  | BH    | 86   | ASP  | 5.9  |
| 30  | DI    | 126  | THR  | 5.9  |
| 53  | B5    | 90   | ALA  | 5.9  |
| 18  | AR    | 20   | GLU  | 5.9  |
| 28  | DG    | 52   | PHE  | 5.9  |
| 13  | CM    | 80   | LEU  | 5.9  |
| 49  | D1    | 24   | THR  | 5.9  |
| 42  | DU    | 21   | LYS  | 5.9  |
| 14  | CN    | 27   | LEU  | 5.9  |
| 29  | BH    | 58   | LEU  | 5.9  |
| 13  | CM    | 46   | SER  | 5.9  |
| 10  | CJ    | 100  | ILE  | 5.9  |
| 53  | B5    | 181  | PHE  | 5.9  |
| 13  | CM    | 109  | ARG  | 5.9  |
| 22  | DA    | 931  | U    | 5.8  |
| 22  | BA    | 885  | C    | 5.8  |
| 19  | CS    | 11   | ILE  | 5.8  |
| 1   | CA    | 1017 | U    | 5.8  |
| 30  | BI    | 8    | TYR  | 5.8  |
| 14  | AN    | 30   | ILE  | 5.8  |
| 22  | BA    | 2173 | A    | 5.8  |
| 53  | B5    | 153  | ILE  | 5.8  |
| 10  | CJ    | 86   | ALA  | 5.8  |
| 39  | DR    | 27   | ILE  | 5.8  |
| 22  | DA    | 2120 | G    | 5.8  |
| 29  | BH    | 137  | GLU  | 5.8  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 27  | DF    | 122  | PHE  | 5.8  |
| 27  | DF    | 54   | ALA  | 5.8  |
| 27  | DF    | 77   | PHE  | 5.8  |
| 27  | DF    | 155  | THR  | 5.8  |
| 22  | DA    | 1066 | U    | 5.8  |
| 30  | BI    | 135  | SER  | 5.8  |
| 9   | CI    | 38   | TYR  | 5.8  |
| 10  | CJ    | 87   | LEU  | 5.8  |
| 10  | CJ    | 82   | LYS  | 5.7  |
| 21  | AU    | 4    | ILE  | 5.7  |
| 29  | BH    | 113  | SER  | 5.7  |
| 30  | DI    | 32   | GLY  | 5.7  |
| 22  | BA    | 2131 | U    | 5.7  |
| 53  | B5    | 206  | LYS  | 5.7  |
| 22  | DA    | 1068 | G    | 5.7  |
| 26  | DE    | 104  | ALA  | 5.7  |
| 30  | BI    | 21   | SER  | 5.7  |
| 27  | DF    | 25   | VAL  | 5.7  |
| 53  | B5    | 152  | GLU  | 5.7  |
| 7   | CG    | 75   | VAL  | 5.7  |
| 42  | BU    | 49   | VAL  | 5.7  |
| 22  | DA    | 2585 | U    | 5.7  |
| 7   | CG    | 77   | SER  | 5.7  |
| 8   | CH    | 2    | SER  | 5.7  |
| 53  | B5    | 128  | LEU  | 5.7  |
| 13  | CM    | 2    | ALA  | 5.7  |
| 17  | AQ    | 20   | SER  | 5.7  |
| 27  | DF    | 23   | ASN  | 5.7  |
| 27  | DF    | 67   | ILE  | 5.7  |
| 30  | DI    | 91   | GLY  | 5.7  |
| 10  | CJ    | 99   | GLN  | 5.7  |
| 29  | BH    | 144  | VAL  | 5.7  |
| 8   | AH    | 2    | SER  | 5.7  |
| 9   | CI    | 64   | TYR  | 5.7  |
| 16  | AP    | 80   | LYS  | 5.7  |
| 29  | BH    | 91   | PHE  | 5.7  |
| 3   | CC    | 193  | TYR  | 5.7  |
| 30  | BI    | 66   | SER  | 5.7  |
| 22  | DA    | 2168 | G    | 5.7  |
| 16  | CP    | 80   | LYS  | 5.6  |
| 19  | CS    | 49   | ILE  | 5.6  |
| 41  | DT    | 34   | VAL  | 5.6  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 2          | AB           | 135        | LEU         | 5.6         |
| 40         | DS           | 92         | ARG         | 5.6         |
| 53         | B5           | 82         | GLU         | 5.6         |
| 2          | AB           | 9          | MET         | 5.6         |
| 7          | CG           | 73         | VAL         | 5.6         |
| 22         | DA           | 1171       | G           | 5.6         |
| 40         | DS           | 84         | ARG         | 5.6         |
| 33         | DL           | 144        | GLU         | 5.6         |
| 19         | CS           | 39         | THR         | 5.6         |
| 30         | DI           | 112        | THR         | 5.6         |
| 42         | DU           | 77         | THR         | 5.6         |
| 22         | BA           | 2125       | G           | 5.6         |
| 30         | DI           | 35         | ILE         | 5.6         |
| 53         | B5           | 172        | ILE         | 5.6         |
| 30         | DI           | 20         | PRO         | 5.6         |
| 42         | BU           | 55         | PRO         | 5.6         |
| 22         | BA           | 2119       | A           | 5.6         |
| 22         | DA           | 1084       | A           | 5.6         |
| 19         | CS           | 48         | THR         | 5.6         |
| 13         | CM           | 47         | GLU         | 5.6         |
| 53         | B5           | 41         | THR         | 5.6         |
| 41         | DT           | 15         | HIS         | 5.5         |
| 53         | B5           | 61         | GLY         | 5.5         |
| 53         | B5           | 121        | MET         | 5.5         |
| 53         | B5           | 212        | SER         | 5.5         |
| 30         | BI           | 68         | THR         | 5.5         |
| 7          | CG           | 18         | PHE         | 5.5         |
| 13         | CM           | 79         | ARG         | 5.5         |
| 30         | DI           | 138        | LEU         | 5.5         |
| 53         | B5           | 144        | GLY         | 5.5         |
| 7          | CG           | 91         | VAL         | 5.5         |
| 27         | DF           | 152        | LEU         | 5.5         |
| 30         | DI           | 43         | ASN         | 5.5         |
| 29         | BH           | 123        | ARG         | 5.5         |
| 7          | CG           | 134        | ALA         | 5.5         |
| 1          | CA           | 209        | U           | 5.5         |
| 41         | DT           | 70         | HIS         | 5.5         |
| 27         | DF           | 51         | ASP         | 5.5         |
| 29         | BH           | 115        | VAL         | 5.5         |
| 53         | B5           | 187        | ALA         | 5.4         |
| 42         | DU           | 48         | PRO         | 5.4         |
| 53         | B5           | 65         | LEU         | 5.4         |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 28  | DG    | 80   | THR  | 5.4  |
| 10  | CJ    | 10   | LEU  | 5.4  |
| 13  | CM    | 106  | ALA  | 5.4  |
| 51  | D3    | 57   | LEU  | 5.4  |
| 22  | DA    | 2175 | C    | 5.4  |
| 29  | BH    | 112  | LYS  | 5.4  |
| 53  | B5    | 38   | PHE  | 5.4  |
| 22  | BA    | 138  | U    | 5.4  |
| 14  | CN    | 29   | ALA  | 5.4  |
| 42  | DU    | 36   | VAL  | 5.4  |
| 9   | CI    | 125  | PRO  | 5.4  |
| 27  | DF    | 26   | MET  | 5.4  |
| 2   | CB    | 130  | THR  | 5.4  |
| 21  | AU    | 38   | TYR  | 5.4  |
| 29  | DH    | 79   | THR  | 5.4  |
| 13  | CM    | 52   | GLN  | 5.4  |
| 14  | CN    | 45   | VAL  | 5.4  |
| 7   | CG    | 53   | ARG  | 5.4  |
| 13  | CM    | 62   | LYS  | 5.4  |
| 28  | DG    | 43   | VAL  | 5.4  |
| 22  | DA    | 2125 | G    | 5.4  |
| 9   | CI    | 89   | GLU  | 5.4  |
| 13  | CM    | 19   | LEU  | 5.4  |
| 17  | AQ    | 83   | VAL  | 5.3  |
| 19  | CS    | 76   | PRO  | 5.3  |
| 14  | CN    | 54   | ASP  | 5.3  |
| 12  | CL    | 124  | ALA  | 5.3  |
| 30  | BI    | 55   | ILE  | 5.3  |
| 22  | BA    | 1065 | U    | 5.3  |
| 41  | DT    | 76   | ARG  | 5.3  |
| 27  | DF    | 22   | TYR  | 5.3  |
| 1   | CA    | 1026 | G    | 5.3  |
| 19  | CS    | 44   | MET  | 5.3  |
| 22  | BA    | 2133 | G    | 5.3  |
| 10  | CJ    | 19   | ASP  | 5.3  |
| 53  | B5    | 137  | LEU  | 5.3  |
| 15  | AO    | 89   | ARG  | 5.3  |
| 32  | DK    | 111  | LYS  | 5.3  |
| 52  | D4    | 8    | LYS  | 5.3  |
| 30  | BI    | 14   | ALA  | 5.3  |
| 19  | AS    | 49   | ILE  | 5.3  |
| 22  | BA    | 2186 | G    | 5.3  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 25         | DD           | 60         | VAL         | 5.3         |
| 28         | DG           | 103        | ILE         | 5.2         |
| 53         | B5           | 164        | PHE         | 5.2         |
| 14         | CN           | 60         | GLN         | 5.2         |
| 46         | DY           | 36         | GLN         | 5.2         |
| 7          | CG           | 59         | LEU         | 5.2         |
| 53         | B5           | 79         | ALA         | 5.2         |
| 46         | DY           | 59         | GLU         | 5.2         |
| 7          | CG           | 79         | ARG         | 5.2         |
| 29         | BH           | 132        | PHE         | 5.2         |
| 30         | DI           | 128        | SER         | 5.2         |
| 22         | DA           | 1172       | C           | 5.2         |
| 22         | DA           | 896        | A           | 5.2         |
| 10         | CJ           | 81         | GLU         | 5.2         |
| 27         | DF           | 29         | PRO         | 5.2         |
| 10         | CJ           | 72         | ARG         | 5.2         |
| 14         | CN           | 47         | LYS         | 5.2         |
| 30         | DI           | 17         | MET         | 5.2         |
| 29         | BH           | 83         | LYS         | 5.2         |
| 22         | DA           | 2797       | U           | 5.2         |
| 30         | BI           | 84         | ALA         | 5.2         |
| 42         | DU           | 71         | ALA         | 5.2         |
| 13         | CM           | 12         | HIS         | 5.2         |
| 1          | CA           | 1021       | A           | 5.1         |
| 19         | CS           | 17         | LYS         | 5.1         |
| 22         | BA           | 1094       | U           | 5.1         |
| 53         | B5           | 192        | ALA         | 5.1         |
| 27         | DF           | 156        | ILE         | 5.1         |
| 53         | B5           | 83         | LYS         | 5.1         |
| 13         | CM           | 55         | THR         | 5.1         |
| 13         | CM           | 86         | TYR         | 5.1         |
| 36         | DO           | 99         | TYR         | 5.1         |
| 46         | BY           | 63         | ALA         | 5.1         |
| 29         | BH           | 131        | SER         | 5.1         |
| 53         | B5           | 169        | THR         | 5.1         |
| 30         | DI           | 10         | LYS         | 5.1         |
| 53         | B5           | 89         | GLU         | 5.1         |
| 27         | BF           | 80         | ARG         | 5.1         |
| 27         | DF           | 80         | ARG         | 5.1         |
| 28         | DG           | 58         | TYR         | 5.1         |
| 53         | B5           | 39         | ASP         | 5.1         |
| 13         | CM           | 31         | LYS         | 5.1         |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 30  | DI    | 15   | ALA  | 5.1  |
| 22  | DA    | 1090 | A    | 5.1  |
| 53  | B5    | 197  | LEU  | 5.1  |
| 22  | BA    | 2106 | U    | 5.1  |
| 30  | BI    | 96   | ASP  | 5.1  |
| 30  | DI    | 12   | GLN  | 5.1  |
| 1   | CA    | 94   | G    | 5.1  |
| 53  | B5    | 50   | ILE  | 5.0  |
| 30  | BI    | 23   | PRO  | 5.0  |
| 53  | B5    | 176  | VAL  | 5.0  |
| 7   | CG    | 78   | ARG  | 5.0  |
| 13  | CM    | 75   | MET  | 5.0  |
| 22  | DA    | 138  | U    | 5.0  |
| 22  | DA    | 1094 | U    | 5.0  |
| 30  | BI    | 78   | VAL  | 5.0  |
| 53  | B5    | 74   | ARG  | 5.0  |
| 22  | DA    | 2172 | U    | 5.0  |
| 7   | CG    | 85   | TYR  | 5.0  |
| 30  | DI    | 92   | LYS  | 5.0  |
| 7   | CG    | 152  | ALA  | 5.0  |
| 30  | DI    | 36   | MET  | 5.0  |
| 9   | AI    | 20   | PHE  | 5.0  |
| 19  | CS    | 68   | GLY  | 5.0  |
| 46  | DY    | 28   | LEU  | 5.0  |
| 22  | DA    | 2173 | A    | 5.0  |
| 22  | DA    | 2176 | A    | 5.0  |
| 29  | BH    | 120  | GLY  | 5.0  |
| 53  | B5    | 188  | ASP  | 5.0  |
| 22  | DA    | 846  | U    | 5.0  |
| 22  | DA    | 2180 | U    | 5.0  |
| 33  | DL    | 101  | ILE  | 5.0  |
| 28  | DG    | 167  | GLU  | 5.0  |
| 1   | AA    | 1534 | A    | 5.0  |
| 22  | DA    | 1048 | A    | 5.0  |
| 22  | BA    | 2146 | C    | 5.0  |
| 22  | BA    | 2105 | U    | 5.0  |
| 14  | CN    | 48   | LEU  | 5.0  |
| 14  | CN    | 11   | VAL  | 4.9  |
| 30  | BI    | 92   | LYS  | 4.9  |
| 30  | DI    | 119  | GLY  | 4.9  |
| 53  | B5    | 126  | SER  | 4.9  |
| 53  | B5    | 222  | SER  | 4.9  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 10  | CJ    | 73   | LEU  | 4.9  |
| 19  | CS    | 13   | LEU  | 4.9  |
| 26  | DE    | 144  | GLU  | 4.9  |
| 30  | DI    | 63   | ALA  | 4.9  |
| 22  | BA    | 2170 | A    | 4.9  |
| 53  | B5    | 225  | ILE  | 4.9  |
| 1   | CA    | 1242 | G    | 4.9  |
| 19  | CS    | 59   | PRO  | 4.9  |
| 52  | D4    | 12   | ARG  | 4.9  |
| 53  | B5    | 53   | ARG  | 4.9  |
| 22  | DA    | 1174 | U    | 4.9  |
| 22  | DA    | 2402 | U    | 4.9  |
| 26  | DE    | 164  | LEU  | 4.9  |
| 22  | BA    | 1063 | G    | 4.9  |
| 13  | CM    | 51   | GLY  | 4.9  |
| 28  | DG    | 26   | ILE  | 4.9  |
| 29  | BH    | 87   | GLU  | 4.9  |
| 7   | CG    | 69   | VAL  | 4.9  |
| 27  | DF    | 143  | TYR  | 4.9  |
| 29  | BH    | 148  | ALA  | 4.9  |
| 19  | CS    | 41   | PHE  | 4.9  |
| 14  | CN    | 35   | ASN  | 4.9  |
| 28  | DG    | 168  | VAL  | 4.8  |
| 27  | DF    | 10   | ASP  | 4.8  |
| 49  | D1    | 36   | LEU  | 4.8  |
| 10  | CJ    | 80   | THR  | 4.8  |
| 3   | CC    | 91   | VAL  | 4.8  |
| 16  | AP    | 81   | ALA  | 4.8  |
| 10  | CJ    | 71   | LEU  | 4.8  |
| 22  | BA    | 1171 | G    | 4.8  |
| 7   | CG    | 148  | ASN  | 4.8  |
| 42  | DU    | 80   | ALA  | 4.8  |
| 30  | DI    | 87   | LYS  | 4.8  |
| 22  | DA    | 1085 | A    | 4.8  |
| 36  | DO    | 117  | PHE  | 4.8  |
| 41  | DT    | 8    | LEU  | 4.8  |
| 28  | DG    | 45   | HIS  | 4.8  |
| 41  | DT    | 43   | ILE  | 4.8  |
| 51  | D3    | 61   | CYS  | 4.8  |
| 13  | CM    | 94   | GLY  | 4.8  |
| 13  | CM    | 114  | LYS  | 4.8  |
| 22  | BA    | 896  | A    | 4.8  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 30  | BI    | 121  | ASP  | 4.8  |
| 53  | B5    | 57   | GLN  | 4.8  |
| 1   | AA    | 87   | C    | 4.8  |
| 48  | D0    | 57   | LYS  | 4.8  |
| 53  | B5    | 54   | ARG  | 4.8  |
| 27  | DF    | 65   | PRO  | 4.8  |
| 53  | B5    | 24   | ASP  | 4.8  |
| 7   | CG    | 72   | THR  | 4.8  |
| 3   | CC    | 79   | LYS  | 4.8  |
| 9   | CI    | 129  | LYS  | 4.8  |
| 13  | CM    | 98   | ARG  | 4.8  |
| 1   | AA    | 844  | G    | 4.8  |
| 30  | DI    | 24   | VAL  | 4.8  |
| 53  | B5    | 75   | VAL  | 4.8  |
| 30  | DI    | 18   | ALA  | 4.8  |
| 42  | DU    | 3    | ALA  | 4.8  |
| 2   | CB    | 67   | ILE  | 4.8  |
| 2   | CB    | 83   | ALA  | 4.7  |
| 3   | CC    | 192  | THR  | 4.7  |
| 48  | D0    | 26   | THR  | 4.7  |
| 13  | CM    | 38   | GLY  | 4.7  |
| 9   | CI    | 58   | VAL  | 4.7  |
| 9   | AI    | 104  | VAL  | 4.7  |
| 13  | CM    | 65   | VAL  | 4.7  |
| 33  | DL    | 89   | VAL  | 4.7  |
| 22  | DA    | 1870 | C    | 4.7  |
| 53  | B5    | 210  | LEU  | 4.7  |
| 13  | AM    | 4    | ILE  | 4.7  |
| 13  | CM    | 58   | ASP  | 4.7  |
| 33  | DL    | 142  | ILE  | 4.7  |
| 53  | B5    | 167  | ASP  | 4.7  |
| 22  | DA    | 12   | U    | 4.7  |
| 14  | CN    | 26   | GLU  | 4.7  |
| 53  | B5    | 99   | GLU  | 4.7  |
| 53  | B5    | 130  | ARG  | 4.7  |
| 29  | BH    | 62   | LEU  | 4.7  |
| 42  | DU    | 63   | ALA  | 4.7  |
| 20  | CT    | 9    | LYS  | 4.7  |
| 22  | DA    | 546  | U    | 4.7  |
| 36  | DO    | 24   | THR  | 4.7  |
| 53  | B5    | 73   | VAL  | 4.7  |
| 2   | CB    | 37   | LYS  | 4.7  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 30  | DI    | 122  | ILE  | 4.7  |
| 53  | B5    | 136  | GLY  | 4.7  |
| 22  | DA    | 1076 | C    | 4.7  |
| 53  | B5    | 195  | ARG  | 4.7  |
| 48  | D0    | 54   | VAL  | 4.7  |
| 36  | DO    | 40   | ILE  | 4.7  |
| 49  | D1    | 52   | ALA  | 4.7  |
| 20  | CT    | 3    | ASN  | 4.7  |
| 11  | AK    | 14   | LYS  | 4.7  |
| 2   | CB    | 136  | MET  | 4.6  |
| 13  | CM    | 43   | VAL  | 4.6  |
| 36  | DO    | 85   | LYS  | 4.6  |
| 9   | CI    | 126  | GLN  | 4.6  |
| 27  | DF    | 31   | VAL  | 4.6  |
| 43  | DV    | 57   | TYR  | 4.6  |
| 40  | DS    | 94   | ASP  | 4.6  |
| 1   | AA    | 85   | U    | 4.6  |
| 13  | CM    | 56   | LEU  | 4.6  |
| 50  | D2    | 42   | LEU  | 4.6  |
| 27  | DF    | 32   | GLU  | 4.6  |
| 29  | BH    | 55   | GLU  | 4.6  |
| 49  | D1    | 53   | LYS  | 4.6  |
| 53  | B5    | 63   | VAL  | 4.6  |
| 7   | CG    | 45   | SER  | 4.6  |
| 19  | CS    | 75   | ALA  | 4.6  |
| 7   | CG    | 15   | ASP  | 4.6  |
| 30  | DI    | 31   | GLN  | 4.6  |
| 36  | DO    | 46   | GLU  | 4.6  |
| 30  | DI    | 86   | ILE  | 4.6  |
| 50  | B2    | 46   | LYS  | 4.6  |
| 7   | CG    | 49   | THR  | 4.6  |
| 13  | CM    | 72   | GLU  | 4.6  |
| 22  | DA    | 1074 | G    | 4.6  |
| 28  | DG    | 57   | GLY  | 4.6  |
| 30  | DI    | 70   | VAL  | 4.6  |
| 30  | BI    | 117  | MET  | 4.6  |
| 2   | AB    | 74   | ARG  | 4.6  |
| 22  | DA    | 1075 | C    | 4.6  |
| 53  | B5    | 211  | ARG  | 4.6  |
| 10  | AJ    | 74   | VAL  | 4.6  |
| 14  | CN    | 34   | VAL  | 4.6  |
| 13  | AM    | 33   | ILE  | 4.6  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 41  | DT    | 42   | GLU  | 4.6  |
| 51  | D3    | 14   | PHE  | 4.6  |
| 27  | DF    | 120  | LYS  | 4.6  |
| 27  | BF    | 74   | VAL  | 4.5  |
| 29  | BH    | 61   | VAL  | 4.5  |
| 34  | DM    | 99   | GLY  | 4.6  |
| 53  | B5    | 124  | VAL  | 4.5  |
| 38  | DQ    | 74   | ILE  | 4.5  |
| 29  | DH    | 15   | LEU  | 4.5  |
| 28  | DG    | 48   | ASN  | 4.5  |
| 22  | DA    | 1064 | C    | 4.5  |
| 1   | AA    | 1537 | U    | 4.5  |
| 19  | CS    | 42   | PRO  | 4.5  |
| 29  | BH    | 64   | ALA  | 4.5  |
| 20  | AT    | 68   | HIS  | 4.5  |
| 26  | DE    | 201  | ALA  | 4.5  |
| 30  | DI    | 127  | ARG  | 4.5  |
| 30  | DI    | 62   | TYR  | 4.5  |
| 27  | DF    | 106  | ILE  | 4.5  |
| 53  | B5    | 145  | THR  | 4.5  |
| 27  | DF    | 41   | GLY  | 4.5  |
| 52  | D4    | 33   | HIS  | 4.5  |
| 22  | DA    | 2109 | U    | 4.5  |
| 32  | DK    | 110  | GLU  | 4.5  |
| 22  | DA    | 885  | C    | 4.5  |
| 22  | DA    | 1606 | C    | 4.5  |
| 7   | CG    | 116  | MET  | 4.5  |
| 3   | CC    | 39   | VAL  | 4.5  |
| 41  | DT    | 55   | VAL  | 4.5  |
| 2   | CB    | 139  | ARG  | 4.5  |
| 30  | DI    | 81   | LYS  | 4.5  |
| 22  | BA    | 2137 | U    | 4.5  |
| 53  | B5    | 135  | ARG  | 4.5  |
| 30  | BI    | 6    | GLN  | 4.5  |
| 40  | DS    | 68   | ASP  | 4.5  |
| 30  | BI    | 71   | THR  | 4.5  |
| 39  | DR    | 29   | THR  | 4.5  |
| 9   | CI    | 90   | TYR  | 4.5  |
| 13  | CM    | 48   | LEU  | 4.4  |
| 44  | DW    | 38   | VAL  | 4.4  |
| 2   | CB    | 9    | MET  | 4.4  |
| 28  | DG    | 111  | HIS  | 4.4  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 53  | B5    | 200  | HIS  | 4.4  |
| 13  | CM    | 71   | ARG  | 4.4  |
| 39  | DR    | 50   | GLY  | 4.4  |
| 19  | CS    | 43   | ASN  | 4.4  |
| 22  | DA    | 1103 | A    | 4.4  |
| 22  | DA    | 2163 | A    | 4.4  |
| 1   | CA    | 1540 | U    | 4.4  |
| 27  | DF    | 176  | PRO  | 4.4  |
| 10  | CJ    | 102  | LEU  | 4.4  |
| 22  | BA    | 2108 | A    | 4.4  |
| 22  | DA    | 1083 | U    | 4.4  |
| 22  | DA    | 2167 | U    | 4.4  |
| 52  | D4    | 9    | LYS  | 4.4  |
| 13  | CM    | 33   | ILE  | 4.4  |
| 40  | DS    | 85   | ILE  | 4.4  |
| 30  | BI    | 91   | GLY  | 4.4  |
| 7   | AG    | 4    | ARG  | 4.4  |
| 53  | B5    | 215  | VAL  | 4.4  |
| 22  | DA    | 1046 | A    | 4.4  |
| 27  | DF    | 173  | PHE  | 4.4  |
| 30  | DI    | 42   | PHE  | 4.4  |
| 48  | D0    | 27   | SER  | 4.4  |
| 27  | DF    | 38   | MET  | 4.4  |
| 30  | BI    | 81   | LYS  | 4.4  |
| 1   | CA    | 1235 | U    | 4.4  |
| 1   | CA    | 983  | A    | 4.4  |
| 30  | DI    | 50   | GLU  | 4.4  |
| 19  | CS    | 28   | LYS  | 4.4  |
| 22  | BA    | 1172 | C    | 4.4  |
| 14  | CN    | 24   | ARG  | 4.4  |
| 28  | DG    | 56   | ASP  | 4.4  |
| 32  | DK    | 89   | ASN  | 4.4  |
| 22  | BA    | 2109 | U    | 4.4  |
| 30  | DI    | 101  | ILE  | 4.4  |
| 53  | B5    | 123  | ALA  | 4.3  |
| 18  | AR    | 51   | TYR  | 4.3  |
| 27  | DF    | 153  | ASP  | 4.3  |
| 2   | AB    | 131  | LYS  | 4.3  |
| 7   | CG    | 43   | VAL  | 4.3  |
| 22  | DA    | 1535 | A    | 4.3  |
| 4   | CD    | 36   | GLN  | 4.3  |
| 2   | CB    | 34   | ALA  | 4.3  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 19         | CS           | 50         | ALA         | 4.3         |
| 2          | CB           | 22         | TYR         | 4.3         |
| 19         | CS           | 12         | ASP         | 4.3         |
| 42         | DU           | 49         | VAL         | 4.3         |
| 30         | BI           | 34         | ASN         | 4.3         |
| 36         | DO           | 63         | LYS         | 4.3         |
| 22         | DA           | 1086       | A           | 4.3         |
| 30         | BI           | 41         | ALA         | 4.3         |
| 30         | BI           | 48         | SER         | 4.3         |
| 29         | BH           | 94         | ILE         | 4.3         |
| 53         | B5           | 101        | ILE         | 4.3         |
| 7          | CG           | 109        | ARG         | 4.3         |
| 10         | CJ           | 89         | ARG         | 4.3         |
| 13         | CM           | 4          | ILE         | 4.3         |
| 13         | CM           | 29         | ARG         | 4.3         |
| 52         | D4           | 29         | ALA         | 4.3         |
| 53         | B5           | 28         | ARG         | 4.3         |
| 22         | DA           | 1087       | G           | 4.3         |
| 2          | CB           | 129        | LEU         | 4.3         |
| 19         | AS           | 31         | LEU         | 4.3         |
| 30         | DI           | 39         | CYS         | 4.3         |
| 33         | DL           | 80         | SER         | 4.3         |
| 2          | CB           | 138        | THR         | 4.2         |
| 7          | CG           | 51         | ALA         | 4.2         |
| 53         | B5           | 196        | ALA         | 4.2         |
| 33         | DL           | 62         | PRO         | 4.2         |
| 24         | DC           | 49         | ILE         | 4.2         |
| 37         | DP           | 84         | ILE         | 4.2         |
| 37         | DP           | 111        | LYS         | 4.2         |
| 22         | BA           | 2151       | U           | 4.2         |
| 27         | DF           | 157        | THR         | 4.2         |
| 53         | B5           | 103        | LYS         | 4.2         |
| 30         | DI           | 7          | ALA         | 4.2         |
| 17         | CQ           | 50         | ASN         | 4.2         |
| 10         | CJ           | 7          | ARG         | 4.2         |
| 39         | DR           | 96         | VAL         | 4.2         |
| 27         | DF           | 60         | ILE         | 4.2         |
| 29         | BH           | 67         | ALA         | 4.2         |
| 2          | CB           | 35         | ARG         | 4.2         |
| 19         | AS           | 39         | THR         | 4.2         |
| 1          | CA           | 1305       | G           | 4.2         |
| 7          | CG           | 80         | VAL         | 4.2         |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 30  | BI    | 15   | ALA  | 4.2  |
| 29  | DH    | 119  | ASN  | 4.2  |
| 7   | CG    | 87   | VAL  | 4.2  |
| 26  | DE    | 28   | VAL  | 4.2  |
| 27  | DF    | 151  | GLY  | 4.2  |
| 1   | AA    | 79   | G    | 4.2  |
| 42  | DU    | 79   | LYS  | 4.2  |
| 22  | DA    | 1049 | C    | 4.2  |
| 53  | B5    | 203  | GLU  | 4.2  |
| 9   | CI    | 124  | ARG  | 4.2  |
| 34  | DM    | 136  | MET  | 4.2  |
| 7   | CG    | 50   | LEU  | 4.2  |
| 30  | BI    | 83   | ALA  | 4.2  |
| 43  | DV    | 32   | GLY  | 4.2  |
| 3   | CC    | 42   | TYR  | 4.2  |
| 16  | AP    | 22   | ALA  | 4.1  |
| 22  | BA    | 1066 | U    | 4.2  |
| 17  | CQ    | 5    | ILE  | 4.1  |
| 22  | DA    | 2121 | G    | 4.1  |
| 49  | D1    | 47   | VAL  | 4.1  |
| 53  | B5    | 204  | GLY  | 4.1  |
| 28  | DG    | 150  | ALA  | 4.1  |
| 42  | DU    | 88   | GLU  | 4.1  |
| 46  | DY    | 56   | LEU  | 4.1  |
| 13  | CM    | 87   | ARG  | 4.1  |
| 33  | DL    | 78   | ARG  | 4.1  |
| 2   | CB    | 132  | LYS  | 4.1  |
| 19  | CS    | 25   | SER  | 4.1  |
| 28  | DG    | 86   | LYS  | 4.1  |
| 1   | CA    | 211  | G    | 4.1  |
| 22  | DA    | 2107 | G    | 4.1  |
| 27  | DF    | 102  | ARG  | 4.1  |
| 44  | DW    | 32   | LEU  | 4.1  |
| 19  | CS    | 64   | ASP  | 4.1  |
| 13  | CM    | 70   | ARG  | 4.1  |
| 19  | AS    | 32   | ARG  | 4.1  |
| 30  | BI    | 26   | PRO  | 4.1  |
| 22  | DA    | 2307 | G    | 4.1  |
| 37  | DP    | 91   | ALA  | 4.1  |
| 28  | DG    | 10   | VAL  | 4.1  |
| 27  | DF    | 148  | ARG  | 4.1  |
| 4   | AD    | 36   | GLN  | 4.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 21  | CU    | 38   | TYR  | 4.1  |
| 22  | DA    | 2119 | A    | 4.1  |
| 10  | CJ    | 8    | ILE  | 4.1  |
| 7   | CG    | 86   | GLN  | 4.1  |
| 9   | AI    | 21   | ILE  | 4.1  |
| 13  | CM    | 17   | ILE  | 4.1  |
| 22  | DA    | 1095 | A    | 4.1  |
| 39  | DR    | 75   | VAL  | 4.1  |
| 53  | B5    | 175  | PRO  | 4.1  |
| 46  | DY    | 4    | LYS  | 4.1  |
| 9   | CI    | 32   | GLN  | 4.1  |
| 22  | DA    | 884  | U    | 4.1  |
| 30  | BI    | 142  | ASP  | 4.0  |
| 27  | DF    | 40   | VAL  | 4.0  |
| 27  | DF    | 89   | VAL  | 4.0  |
| 19  | AS    | 74   | PHE  | 4.0  |
| 22  | BA    | 2309 | A    | 4.0  |
| 22  | DA    | 2123 | G    | 4.0  |
| 1   | CA    | 999  | C    | 4.0  |
| 30  | DI    | 45   | LYS  | 4.0  |
| 28  | DG    | 59   | ALA  | 4.0  |
| 30  | DI    | 84   | ALA  | 4.0  |
| 4   | AD    | 25   | VAL  | 4.0  |
| 13  | CM    | 61   | ALA  | 4.0  |
| 13  | AM    | 115  | PRO  | 4.0  |
| 7   | CG    | 103  | TRP  | 4.0  |
| 26  | DE    | 33   | VAL  | 4.0  |
| 35  | DN    | 76   | VAL  | 4.0  |
| 49  | D1    | 48   | ILE  | 4.0  |
| 50  | D2    | 33   | ARG  | 4.0  |
| 40  | DS    | 3    | THR  | 4.0  |
| 14  | CN    | 2    | ALA  | 4.0  |
| 7   | CG    | 76   | LYS  | 4.0  |
| 13  | CM    | 16   | VAL  | 4.0  |
| 53  | B5    | 193  | PHE  | 4.0  |
| 6   | AF    | 95   | ALA  | 4.0  |
| 29  | DH    | 140  | ALA  | 4.0  |
| 30  | DI    | 134  | ARG  | 4.0  |
| 10  | CJ    | 75   | ASP  | 4.0  |
| 33  | DL    | 106  | GLU  | 4.0  |
| 14  | CN    | 44   | ALA  | 4.0  |
| 22  | DA    | 2165 | C    | 4.0  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 22  | BA    | 139  | U    | 4.0  |
| 22  | BA    | 884  | U    | 4.0  |
| 27  | DF    | 149  | VAL  | 4.0  |
| 42  | DU    | 13   | VAL  | 4.0  |
| 1   | CA    | 207  | C    | 4.0  |
| 14  | CN    | 50   | THR  | 4.0  |
| 30  | BI    | 56   | PRO  | 4.0  |
| 35  | DN    | 29   | VAL  | 4.0  |
| 4   | AD    | 28   | ILE  | 4.0  |
| 27  | DF    | 111  | ILE  | 4.0  |
| 49  | D1    | 34   | LEU  | 4.0  |
| 33  | DL    | 108  | ALA  | 4.0  |
| 52  | D4    | 1    | MET  | 4.0  |
| 1   | AA    | 81   | A    | 3.9  |
| 7   | CG    | 84   | THR  | 3.9  |
| 7   | CG    | 141  | VAL  | 3.9  |
| 52  | D4    | 26   | ILE  | 3.9  |
| 32  | DK    | 112  | PHE  | 3.9  |
| 53  | B5    | 133  | GLY  | 3.9  |
| 28  | DG    | 27   | LYS  | 3.9  |
| 2   | AB    | 139  | ARG  | 3.9  |
| 9   | CI    | 20   | PHE  | 3.9  |
| 10  | CJ    | 92   | LEU  | 3.9  |
| 29  | DH    | 54   | LEU  | 3.9  |
| 46  | DY    | 37   | LEU  | 3.9  |
| 22  | DA    | 2157 | G    | 3.9  |
| 28  | DG    | 151  | TYR  | 3.9  |
| 33  | DL    | 121  | THR  | 3.9  |
| 33  | DL    | 70   | LYS  | 3.9  |
| 53  | B5    | 184  | GLU  | 3.9  |
| 53  | B5    | 220  | GLY  | 3.9  |
| 9   | CI    | 7    | TYR  | 3.9  |
| 30  | DI    | 125  | MET  | 3.9  |
| 22  | DA    | 1407 | G    | 3.9  |
| 53  | B5    | 102  | GLN  | 3.9  |
| 13  | CM    | 24   | GLY  | 3.9  |
| 1   | AA    | 1492 | A    | 3.9  |
| 29  | DH    | 74   | ALA  | 3.9  |
| 30  | BI    | 17   | MET  | 3.9  |
| 30  | BI    | 95   | LYS  | 3.9  |
| 42  | DU    | 47   | LYS  | 3.9  |
| 17  | CQ    | 23   | VAL  | 3.9  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 22  | DA    | 2127 | G    | 3.9  |
| 26  | DE    | 126  | VAL  | 3.9  |
| 14  | CN    | 23   | LYS  | 3.9  |
| 48  | D0    | 34   | SER  | 3.9  |
| 28  | DG    | 9    | VAL  | 3.9  |
| 29  | BH    | 109  | GLU  | 3.9  |
| 30  | DI    | 123  | GLU  | 3.9  |
| 28  | DG    | 112  | PRO  | 3.9  |
| 26  | DE    | 143  | LEU  | 3.9  |
| 33  | DL    | 49   | GLY  | 3.9  |
| 53  | B5    | 49   | GLY  | 3.9  |
| 26  | DE    | 17   | THR  | 3.9  |
| 7   | CG    | 137  | LYS  | 3.9  |
| 14  | CN    | 12   | LYS  | 3.9  |
| 17  | CQ    | 53   | CYS  | 3.9  |
| 3   | CC    | 77   | ILE  | 3.9  |
| 10  | AJ    | 75   | ASP  | 3.9  |
| 27  | DF    | 27   | GLN  | 3.9  |
| 28  | DG    | 77   | ILE  | 3.9  |
| 27  | DF    | 158  | THR  | 3.9  |
| 14  | CN    | 10   | GLU  | 3.9  |
| 22  | DA    | 1173 | U    | 3.9  |
| 29  | DH    | 130  | VAL  | 3.9  |
| 42  | BU    | 54   | GLN  | 3.9  |
| 19  | AS    | 3    | ARG  | 3.9  |
| 30  | DI    | 65   | ARG  | 3.9  |
| 33  | DL    | 82   | LEU  | 3.9  |
| 33  | DL    | 132  | ARG  | 3.9  |
| 46  | DY    | 54   | LYS  | 3.9  |
| 46  | DY    | 14   | LEU  | 3.9  |
| 43  | DV    | 74   | ALA  | 3.9  |
| 9   | CI    | 127  | PHE  | 3.8  |
| 10  | CJ    | 90   | LEU  | 3.8  |
| 13  | AM    | 63   | PHE  | 3.8  |
| 6   | AF    | 92   | THR  | 3.8  |
| 10  | CJ    | 34   | ALA  | 3.8  |
| 27  | DF    | 45   | ALA  | 3.8  |
| 30  | BI    | 120  | ALA  | 3.8  |
| 30  | DI    | 94   | ASN  | 3.8  |
| 10  | CJ    | 20   | GLN  | 3.8  |
| 10  | CJ    | 35   | GLN  | 3.8  |
| 22  | DA    | 653  | U    | 3.8  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 30  | DI    | 102  | SER  | 3.8  |
| 46  | DY    | 7    | ARG  | 3.8  |
| 41  | DT    | 75   | GLY  | 3.8  |
| 27  | DF    | 175  | PHE  | 3.8  |
| 13  | AM    | 31   | LYS  | 3.8  |
| 19  | AS    | 55   | ARG  | 3.8  |
| 7   | CG    | 8    | GLY  | 3.8  |
| 41  | DT    | 60   | THR  | 3.8  |
| 22  | DA    | 1104 | C    | 3.8  |
| 27  | DF    | 174  | ASP  | 3.8  |
| 41  | DT    | 74   | ILE  | 3.8  |
| 2   | AB    | 132  | LYS  | 3.8  |
| 42  | DU    | 19   | LYS  | 3.8  |
| 12  | CL    | 25   | GLU  | 3.8  |
| 2   | CB    | 225  | ARG  | 3.8  |
| 13  | AM    | 5    | ALA  | 3.8  |
| 3   | CC    | 158  | GLY  | 3.8  |
| 2   | AB    | 88   | ASP  | 3.8  |
| 2   | AB    | 221  | VAL  | 3.8  |
| 28  | DG    | 84   | THR  | 3.8  |
| 29  | BH    | 142  | VAL  | 3.8  |
| 10  | CJ    | 27   | GLU  | 3.8  |
| 29  | BH    | 149  | GLU  | 3.8  |
| 10  | CJ    | 45   | ARG  | 3.8  |
| 21  | AU    | 23   | CYS  | 3.8  |
| 1   | AA    | 82   | G    | 3.8  |
| 11  | CK    | 126  | LYS  | 3.8  |
| 22  | DA    | 277  | G    | 3.8  |
| 22  | DA    | 139  | U    | 3.8  |
| 42  | DU    | 29   | LEU  | 3.8  |
| 13  | CM    | 36   | ALA  | 3.8  |
| 30  | DI    | 30   | GLN  | 3.8  |
| 1   | CA    | 1006 | G    | 3.8  |
| 22  | DA    | 895  | U    | 3.8  |
| 36  | DO    | 92   | PHE  | 3.8  |
| 42  | BU    | 53   | ASN  | 3.8  |
| 19  | CS    | 63   | THR  | 3.8  |
| 13  | CM    | 103  | LYS  | 3.8  |
| 43  | DV    | 94   | ALA  | 3.8  |
| 7   | CG    | 17   | LYS  | 3.8  |
| 22  | DA    | 878  | A    | 3.8  |
| 17  | AQ    | 5    | ILE  | 3.8  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 13  | AM    | 114  | LYS  | 3.7  |
| 22  | DA    | 2181 | U    | 3.7  |
| 51  | D3    | 58   | VAL  | 3.8  |
| 26  | DE    | 12   | LEU  | 3.7  |
| 39  | DR    | 26   | ASP  | 3.7  |
| 50  | D2    | 46   | LYS  | 3.7  |
| 52  | D4    | 20   | ASP  | 3.7  |
| 22  | DA    | 1106 | G    | 3.7  |
| 53  | B5    | 43   | GLU  | 3.7  |
| 41  | DT    | 47   | VAL  | 3.7  |
| 33  | DL    | 79   | LEU  | 3.7  |
| 42  | DU    | 14   | LEU  | 3.7  |
| 1   | CA    | 844  | G    | 3.7  |
| 22  | DA    | 1063 | G    | 3.7  |
| 37  | DP    | 92   | VAL  | 3.7  |
| 27  | DF    | 142  | ASP  | 3.7  |
| 11  | CK    | 43   | GLY  | 3.7  |
| 2   | AB    | 226  | SER  | 3.7  |
| 7   | CG    | 83   | SER  | 3.7  |
| 9   | AI    | 32   | GLN  | 3.7  |
| 30  | BI    | 118  | THR  | 3.7  |
| 53  | B5    | 22   | THR  | 3.7  |
| 36  | DO    | 51   | ALA  | 3.7  |
| 27  | DF    | 12   | VAL  | 3.7  |
| 13  | AM    | 19   | LEU  | 3.7  |
| 22  | BA    | 2128 | G    | 3.7  |
| 36  | DO    | 26   | LEU  | 3.7  |
| 37  | DP    | 110  | ILE  | 3.7  |
| 22  | DA    | 2903 | U    | 3.7  |
| 42  | BU    | 52   | LEU  | 3.7  |
| 2   | CB    | 36   | ASN  | 3.7  |
| 20  | CT    | 71   | LYS  | 3.7  |
| 13  | CM    | 115  | PRO  | 3.7  |
| 14  | CN    | 30   | ILE  | 3.7  |
| 22  | DA    | 1044 | C    | 3.7  |
| 28  | DG    | 102  | VAL  | 3.7  |
| 17  | CQ    | 6    | ARG  | 3.7  |
| 29  | DH    | 123  | ARG  | 3.7  |
| 30  | BI    | 39   | CYS  | 3.7  |
| 16  | CP    | 47   | GLU  | 3.7  |
| 22  | DA    | 1058 | U    | 3.7  |
| 22  | DA    | 2305 | U    | 3.7  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 30  | DI    | 51   | LYS  | 3.7  |
| 36  | DO    | 56   | LYS  | 3.7  |
| 22  | DA    | 2112 | G    | 3.7  |
| 27  | DF    | 172  | ALA  | 3.7  |
| 46  | DY    | 16   | THR  | 3.7  |
| 10  | CJ    | 26   | VAL  | 3.7  |
| 45  | DX    | 11   | ARG  | 3.7  |
| 29  | BH    | 122  | LEU  | 3.7  |
| 22  | DA    | 2118 | U    | 3.7  |
| 1   | CA    | 1271 | A    | 3.7  |
| 1   | CA    | 79   | G    | 3.7  |
| 2   | CB    | 152  | LYS  | 3.7  |
| 28  | DG    | 40   | ALA  | 3.7  |
| 30  | DI    | 44   | ALA  | 3.7  |
| 27  | DF    | 117  | LEU  | 3.7  |
| 22  | DA    | 343  | C    | 3.7  |
| 33  | DL    | 87   | GLY  | 3.7  |
| 53  | B5    | 125  | GLY  | 3.7  |
| 22  | DA    | 613  | A    | 3.7  |
| 28  | DG    | 20   | ASN  | 3.7  |
| 9   | AI    | 17   | ALA  | 3.7  |
| 42  | BU    | 51   | ALA  | 3.7  |
| 19  | AS    | 56   | GLN  | 3.7  |
| 13  | CM    | 108  | THR  | 3.7  |
| 22  | DA    | 1211 | C    | 3.6  |
| 27  | DF    | 95   | ARG  | 3.6  |
| 45  | DX    | 50   | ARG  | 3.6  |
| 27  | DF    | 164  | GLU  | 3.6  |
| 13  | CM    | 73   | ILE  | 3.6  |
| 17  | CQ    | 8    | LEU  | 3.6  |
| 29  | DH    | 58   | LEU  | 3.6  |
| 10  | CJ    | 23   | ALA  | 3.6  |
| 13  | AM    | 3    | ARG  | 3.6  |
| 1   | CA    | 950  | U    | 3.6  |
| 2   | CB    | 226  | SER  | 3.6  |
| 46  | DY    | 24   | GLU  | 3.6  |
| 1   | CA    | 988  | G    | 3.6  |
| 30  | BI    | 10   | LYS  | 3.6  |
| 53  | B5    | 205  | ALA  | 3.6  |
| 28  | DG    | 104  | ASN  | 3.6  |
| 13  | CM    | 101  | ARG  | 3.6  |
| 14  | CN    | 57   | PRO  | 3.6  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 20  | AT    | 4    | ILE  | 3.6  |
| 1   | CA    | 1004 | A    | 3.6  |
| 22  | DA    | 877  | A    | 3.6  |
| 53  | B5    | 88   | GLU  | 3.6  |
| 19  | CS    | 47   | LEU  | 3.6  |
| 27  | DF    | 131  | GLY  | 3.6  |
| 9   | CI    | 39   | PHE  | 3.6  |
| 13  | CM    | 89   | LEU  | 3.6  |
| 22  | DA    | 331  | C    | 3.6  |
| 26  | DE    | 103  | GLY  | 3.6  |
| 29  | BH    | 66   | ASN  | 3.6  |
| 30  | BI    | 98   | VAL  | 3.6  |
| 30  | DI    | 13   | VAL  | 3.6  |
| 1   | CA    | 82   | G    | 3.6  |
| 1   | CA    | 1007 | U    | 3.6  |
| 30  | DI    | 105  | GLN  | 3.6  |
| 7   | CG    | 5    | ARG  | 3.6  |
| 16  | CP    | 39   | PHE  | 3.6  |
| 21  | AU    | 7    | ARG  | 3.6  |
| 44  | DW    | 25   | ARG  | 3.6  |
| 13  | CM    | 44   | LYS  | 3.6  |
| 30  | DI    | 100  | LYS  | 3.6  |
| 35  | DN    | 28   | LEU  | 3.6  |
| 36  | DO    | 22   | GLY  | 3.6  |
| 53  | B5    | 120  | VAL  | 3.6  |
| 22  | DA    | 2110 | G    | 3.6  |
| 35  | DN    | 63   | ARG  | 3.6  |
| 27  | DF    | 91   | LEU  | 3.6  |
| 21  | AU    | 9    | ASN  | 3.6  |
| 53  | B5    | 51   | ASP  | 3.6  |
| 22  | DA    | 1105 | U    | 3.6  |
| 50  | D2    | 1    | MET  | 3.6  |
| 26  | DE    | 2    | GLU  | 3.6  |
| 22  | BA    | 1067 | A    | 3.6  |
| 42  | DU    | 5    | ILE  | 3.6  |
| 30  | DI    | 111  | GLN  | 3.6  |
| 24  | DC    | 242  | LYS  | 3.5  |
| 2   | AB    | 134  | ALA  | 3.5  |
| 27  | BF    | 76   | GLY  | 3.5  |
| 28  | DG    | 21   | GLY  | 3.5  |
| 6   | AF    | 36   | ILE  | 3.5  |
| 13  | CM    | 9    | ILE  | 3.5  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 22  | BA    | 1847 | A    | 3.5  |
| 7   | CG    | 131  | LYS  | 3.5  |
| 49  | D1    | 38   | LYS  | 3.5  |
| 22  | BA    | 546  | U    | 3.5  |
| 22  | BA    | 1925 | C    | 3.5  |
| 7   | CG    | 132  | GLY  | 3.5  |
| 29  | BH    | 84   | ALA  | 3.5  |
| 1   | CA    | 1023 | U    | 3.5  |
| 52  | D4    | 16   | ILE  | 3.5  |
| 30  | DI    | 64   | ASP  | 3.5  |
| 1   | CA    | 1296 | C    | 3.5  |
| 9   | CI    | 117  | GLY  | 3.5  |
| 22  | DA    | 1043 | C    | 3.5  |
| 28  | DG    | 17   | VAL  | 3.5  |
| 46  | DY    | 49   | ASP  | 3.5  |
| 19  | CS    | 37   | ARG  | 3.5  |
| 42  | DU    | 90   | GLY  | 3.5  |
| 3   | CC    | 146  | ALA  | 3.5  |
| 29  | BH    | 59   | ALA  | 3.5  |
| 30  | DI    | 106  | LEU  | 3.5  |
| 13  | AM    | 25   | VAL  | 3.5  |
| 14  | AN    | 21   | PHE  | 3.5  |
| 33  | DL    | 81   | ASP  | 3.5  |
| 30  | BI    | 20   | PRO  | 3.5  |
| 9   | AI    | 90   | TYR  | 3.5  |
| 30  | BI    | 104  | ALA  | 3.5  |
| 26  | DE    | 129  | PRO  | 3.5  |
| 42  | DU    | 32   | GLY  | 3.5  |
| 30  | DI    | 19   | ASN  | 3.5  |
| 17  | AQ    | 4    | LYS  | 3.5  |
| 27  | DF    | 144  | ASP  | 3.5  |
| 9   | CI    | 4    | ASN  | 3.5  |
| 25  | DD    | 55   | LYS  | 3.5  |
| 27  | BF    | 72   | LYS  | 3.5  |
| 27  | DF    | 88   | LYS  | 3.5  |
| 42  | DU    | 40   | ASN  | 3.5  |
| 36  | DO    | 21   | LEU  | 3.5  |
| 13  | CM    | 77   | ILE  | 3.5  |
| 14  | CN    | 42   | TRP  | 3.4  |
| 28  | DG    | 176  | LYS  | 3.4  |
| 52  | D4    | 15   | LYS  | 3.4  |
| 7   | CG    | 123  | GLU  | 3.4  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 19  | AS    | 33   | THR  | 3.4  |
| 41  | DT    | 92   | ASN  | 3.4  |
| 44  | BW    | 10   | THR  | 3.4  |
| 46  | DY    | 63   | ALA  | 3.4  |
| 29  | DH    | 61   | VAL  | 3.4  |
| 30  | BI    | 38   | PHE  | 3.4  |
| 1   | AA    | 845  | A    | 3.4  |
| 19  | AS    | 9    | PRO  | 3.4  |
| 22  | BA    | 277  | G    | 3.4  |
| 30  | DI    | 108  | GLU  | 3.4  |
| 19  | CS    | 14   | HIS  | 3.4  |
| 41  | DT    | 87   | LEU  | 3.4  |
| 3   | CC    | 196  | ILE  | 3.4  |
| 14  | CN    | 22   | ALA  | 3.4  |
| 28  | DG    | 92   | VAL  | 3.4  |
| 30  | BI    | 140  | VAL  | 3.4  |
| 33  | DL    | 66   | PHE  | 3.4  |
| 22  | DA    | 2300 | C    | 3.4  |
| 7   | CG    | 70   | ARG  | 3.4  |
| 14  | AN    | 55   | SER  | 3.4  |
| 22  | DA    | 1069 | A    | 3.4  |
| 13  | CM    | 105  | ASN  | 3.4  |
| 17  | CQ    | 21   | ILE  | 3.4  |
| 22  | BA    | 1093 | G    | 3.4  |
| 36  | DO    | 113  | ALA  | 3.4  |
| 46  | DY    | 30   | MET  | 3.4  |
| 27  | DF    | 37   | ASN  | 3.4  |
| 1   | CA    | 1320 | C    | 3.4  |
| 27  | DF    | 170  | LEU  | 3.4  |
| 22  | DA    | 2308 | G    | 3.4  |
| 26  | DE    | 21   | ARG  | 3.4  |
| 29  | DH    | 139  | PHE  | 3.4  |
| 9   | CI    | 120  | LYS  | 3.4  |
| 33  | DL    | 13   | LYS  | 3.4  |
| 40  | DS    | 19   | LEU  | 3.4  |
| 44  | DW    | 59   | LEU  | 3.4  |
| 27  | BF    | 79   | ILE  | 3.4  |
| 30  | DI    | 117  | MET  | 3.4  |
| 47  | DZ    | 48   | ILE  | 3.4  |
| 22  | BA    | 1175 | A    | 3.4  |
| 34  | DM    | 80   | VAL  | 3.4  |
| 42  | DU    | 53   | ASN  | 3.4  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 26         | DE           | 64         | GLY         | 3.4         |
| 37         | DP           | 20         | PHE         | 3.4         |
| 22         | BA           | 1087       | G           | 3.4         |
| 22         | BA           | 2885       | G           | 3.4         |
| 1          | AA           | 88         | U           | 3.4         |
| 1          | AA           | 1031       | C           | 3.4         |
| 1          | CA           | 1317       | C           | 3.4         |
| 22         | DA           | 1045       | C           | 3.4         |
| 28         | DG           | 54         | PRO         | 3.4         |
| 33         | DL           | 3          | LEU         | 3.4         |
| 33         | DL           | 61         | LEU         | 3.4         |
| 19         | CS           | 40         | ILE         | 3.4         |
| 45         | DX           | 18         | ARG         | 3.4         |
| 2          | CB           | 33         | GLY         | 3.4         |
| 7          | CG           | 122        | ASN         | 3.4         |
| 22         | DA           | 345        | A           | 3.4         |
| 30         | BI           | 16         | GLY         | 3.4         |
| 42         | BU           | 56         | GLY         | 3.4         |
| 53         | B5           | 185        | LYS         | 3.4         |
| 22         | DA           | 883        | G           | 3.4         |
| 6          | CF           | 39         | LEU         | 3.4         |
| 22         | DA           | 1072       | C           | 3.4         |
| 29         | BH           | 73         | ASN         | 3.4         |
| 30         | DI           | 97         | LYS         | 3.4         |
| 43         | DV           | 56         | PHE         | 3.4         |
| 9          | CI           | 37         | GLN         | 3.4         |
| 22         | DA           | 1729       | U           | 3.4         |
| 27         | DF           | 133        | ARG         | 3.4         |
| 46         | DY           | 19         | LEU         | 3.4         |
| 37         | DP           | 35         | GLY         | 3.4         |
| 39         | DR           | 66         | HIS         | 3.4         |
| 43         | DV           | 67         | GLY         | 3.4         |
| 53         | B5           | 129        | GLY         | 3.4         |
| 53         | B5           | 58         | ASN         | 3.4         |
| 7          | CG           | 143        | ARG         | 3.3         |
| 9          | CI           | 33         | ARG         | 3.3         |
| 30         | BI           | 138        | LEU         | 3.3         |
| 41         | DT           | 85         | VAL         | 3.3         |
| 1          | CA           | 1028       | C           | 3.3         |
| 22         | DA           | 1107       | G           | 3.3         |
| 22         | DA           | 1170       | C           | 3.3         |
| 27         | DF           | 66         | LEU         | 3.3         |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 7   | AG    | 80   | VAL  | 3.3  |
| 9   | CI    | 44   | ALA  | 3.3  |
| 30  | BI    | 49   | ILE  | 3.3  |
| 44  | DW    | 23   | VAL  | 3.3  |
| 29  | BH    | 82   | SER  | 3.3  |
| 53  | B5    | 191  | ARG  | 3.3  |
| 22  | DA    | 882  | G    | 3.3  |
| 11  | AK    | 111  | THR  | 3.3  |
| 25  | DD    | 133  | THR  | 3.3  |
| 29  | DH    | 6    | LEU  | 3.3  |
| 13  | CM    | 40   | ALA  | 3.3  |
| 22  | DA    | 1089 | A    | 3.3  |
| 25  | DD    | 87   | GLY  | 3.3  |
| 26  | DE    | 128  | ALA  | 3.3  |
| 40  | DS    | 110  | ARG  | 3.3  |
| 50  | D2    | 22   | MET  | 3.3  |
| 53  | B5    | 56   | ASP  | 3.3  |
| 40  | DS    | 69   | LEU  | 3.3  |
| 9   | AI    | 79   | ILE  | 3.3  |
| 10  | CJ    | 41   | PRO  | 3.3  |
| 30  | DI    | 27   | ALA  | 3.3  |
| 39  | DR    | 63   | VAL  | 3.3  |
| 53  | B5    | 221  | PRO  | 3.3  |
| 22  | BA    | 892  | A    | 3.3  |
| 14  | CN    | 58   | SER  | 3.3  |
| 29  | DH    | 135  | HIS  | 3.3  |
| 43  | DV    | 41   | GLU  | 3.3  |
| 9   | CI    | 5    | GLN  | 3.3  |
| 27  | DF    | 36   | LEU  | 3.3  |
| 1   | CA    | 989  | U    | 3.3  |
| 22  | DA    | 1460 | U    | 3.3  |
| 22  | DA    | 1179 | G    | 3.3  |
| 3   | CC    | 71   | ALA  | 3.3  |
| 14  | AN    | 36   | ALA  | 3.3  |
| 30  | DI    | 49   | ILE  | 3.3  |
| 39  | DR    | 99   | THR  | 3.3  |
| 7   | CG    | 14   | PRO  | 3.3  |
| 30  | DI    | 33   | VAL  | 3.3  |
| 1   | CA    | 1274 | A    | 3.3  |
| 22  | DA    | 2170 | A    | 3.3  |
| 13  | CM    | 30   | SER  | 3.3  |
| 19  | CS    | 38   | SER  | 3.3  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 49  | D1    | 18   | GLY  | 3.3  |
| 20  | CT    | 41   | ALA  | 3.3  |
| 26  | DE    | 23   | PHE  | 3.3  |
| 29  | BH    | 139  | PHE  | 3.3  |
| 22  | DA    | 1071 | G    | 3.3  |
| 18  | AR    | 74   | HIS  | 3.3  |
| 27  | BF    | 78   | LYS  | 3.3  |
| 27  | DF    | 69   | LYS  | 3.3  |
| 7   | CG    | 23   | LEU  | 3.3  |
| 20  | CT    | 24   | ARG  | 3.3  |
| 27  | DF    | 50   | LEU  | 3.3  |
| 29  | DH    | 12   | LEU  | 3.3  |
| 45  | DX    | 35   | SER  | 3.3  |
| 1   | CA    | 1027 | C    | 3.3  |
| 26  | DE    | 14   | VAL  | 3.3  |
| 38  | DQ    | 118  | ALA  | 3.3  |
| 53  | B5    | 47   | LYS  | 3.3  |
| 2   | CB    | 213  | TYR  | 3.3  |
| 5   | CE    | 151  | GLU  | 3.3  |
| 22  | BA    | 2402 | U    | 3.3  |
| 36  | DO    | 60   | GLU  | 3.3  |
| 53  | B5    | 23   | ILE  | 3.3  |
| 9   | AI    | 19   | VAL  | 3.3  |
| 28  | DG    | 136  | ALA  | 3.3  |
| 24  | DC    | 47   | GLY  | 3.3  |
| 22  | DA    | 2106 | U    | 3.2  |
| 53  | B5    | 163  | GLU  | 3.2  |
| 10  | AJ    | 36   | VAL  | 3.2  |
| 29  | BH    | 63   | ALA  | 3.2  |
| 28  | DG    | 170  | ARG  | 3.2  |
| 15  | CO    | 25   | THR  | 3.2  |
| 39  | DR    | 32   | THR  | 3.2  |
| 3   | CC    | 144  | LEU  | 3.2  |
| 13  | CM    | 54   | ASP  | 3.2  |
| 33  | DL    | 19   | LEU  | 3.2  |
| 17  | CQ    | 20   | SER  | 3.2  |
| 22  | DA    | 2116 | G    | 3.2  |
| 32  | DK    | 14   | SER  | 3.2  |
| 3   | CC    | 92   | ALA  | 3.2  |
| 7   | CG    | 61   | ALA  | 3.2  |
| 13  | CM    | 37   | ALA  | 3.2  |
| 38  | DQ    | 2    | ALA  | 3.2  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 22  | DA    | 2310 | C    | 3.2  |
| 28  | DG    | 37   | LEU  | 3.2  |
| 5   | AE    | 31   | PHE  | 3.2  |
| 18  | CR    | 74   | HIS  | 3.2  |
| 30  | BI    | 94   | ASN  | 3.2  |
| 39  | DR    | 43   | ASN  | 3.2  |
| 53  | B5    | 150  | ILE  | 3.2  |
| 26  | DE    | 11   | ALA  | 3.2  |
| 22  | DA    | 914  | G    | 3.2  |
| 12  | AL    | 25   | GLU  | 3.2  |
| 29  | BH    | 90   | LEU  | 3.2  |
| 36  | DO    | 62   | LEU  | 3.2  |
| 36  | DO    | 93   | ASP  | 3.2  |
| 3   | CC    | 127  | ARG  | 3.2  |
| 44  | DW    | 78   | LYS  | 3.2  |
| 1   | CA    | 206  | C    | 3.2  |
| 26  | DE    | 131  | THR  | 3.2  |
| 27  | DF    | 150  | ARG  | 3.2  |
| 7   | CG    | 42   | ILE  | 3.2  |
| 52  | D4    | 23   | ILE  | 3.2  |
| 10  | CJ    | 36   | VAL  | 3.2  |
| 13  | CM    | 25   | VAL  | 3.2  |
| 42  | DU    | 28   | VAL  | 3.2  |
| 42  | DU    | 76   | ALA  | 3.2  |
| 48  | D0    | 56   | ALA  | 3.2  |
| 1   | CA    | 1217 | C    | 3.2  |
| 30  | BI    | 119  | GLY  | 3.2  |
| 33  | DL    | 139  | GLY  | 3.2  |
| 42  | BU    | 48   | PRO  | 3.2  |
| 51  | D3    | 52   | LYS  | 3.2  |
| 4   | CD    | 27   | ALA  | 3.2  |
| 6   | AF    | 96   | VAL  | 3.2  |
| 26  | DE    | 32   | VAL  | 3.2  |
| 27  | DF    | 13   | VAL  | 3.2  |
| 7   | CG    | 139  | GLU  | 3.2  |
| 28  | DG    | 82   | GLY  | 3.2  |
| 13  | CM    | 96   | PRO  | 3.2  |
| 13  | CM    | 11   | ASP  | 3.2  |
| 22  | DA    | 2306 | C    | 3.2  |
| 1   | CA    | 1019 | A    | 3.2  |
| 22  | DA    | 866  | A    | 3.2  |
| 7   | CG    | 58   | GLU  | 3.2  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 17  | CQ    | 78   | VAL  | 3.2  |
| 30  | DI    | 104  | ALA  | 3.2  |
| 36  | DO    | 103  | VAL  | 3.2  |
| 25  | DD    | 59   | ARG  | 3.2  |
| 27  | DF    | 93   | GLY  | 3.2  |
| 37  | BP    | 2    | SER  | 3.2  |
| 41  | DT    | 71   | GLY  | 3.2  |
| 27  | DF    | 17   | MET  | 3.2  |
| 53  | B5    | 186  | LEU  | 3.2  |
| 46  | DY    | 13   | GLU  | 3.2  |
| 15  | CO    | 89   | ARG  | 3.2  |
| 21  | AU    | 21   | ARG  | 3.2  |
| 29  | DH    | 148  | ALA  | 3.2  |
| 30  | BI    | 58   | VAL  | 3.2  |
| 23  | DB    | 117  | G    | 3.2  |
| 13  | CM    | 76   | SER  | 3.2  |
| 37  | DP    | 85   | SER  | 3.2  |
| 53  | B5    | 71   | LYS  | 3.2  |
| 41  | DT    | 1    | MET  | 3.2  |
| 22  | DA    | 2150 | C    | 3.2  |
| 11  | AK    | 129  | VAL  | 3.1  |
| 10  | CJ    | 30   | LYS  | 3.1  |
| 41  | DT    | 35   | ALA  | 3.1  |
| 49  | D1    | 37   | LYS  | 3.1  |
| 36  | DO    | 61   | GLN  | 3.1  |
| 41  | DT    | 72   | GLN  | 3.1  |
| 52  | D4    | 35   | GLN  | 3.1  |
| 1   | CA    | 202  | G    | 3.1  |
| 22  | DA    | 356  | G    | 3.1  |
| 7   | AG    | 59   | LEU  | 3.1  |
| 36  | DO    | 106  | LEU  | 3.1  |
| 46  | DY    | 10   | SER  | 3.1  |
| 27  | DF    | 6    | ASP  | 3.1  |
| 7   | CG    | 4    | ARG  | 3.1  |
| 10  | CJ    | 16   | ARG  | 3.1  |
| 25  | DD    | 154  | LYS  | 3.1  |
| 53  | B5    | 178  | LYS  | 3.1  |
| 1   | AA    | 91   | U    | 3.1  |
| 34  | DM    | 79   | ALA  | 3.1  |
| 39  | DR    | 42   | ALA  | 3.1  |
| 41  | DT    | 41   | ALA  | 3.1  |
| 30  | BI    | 89   | GLY  | 3.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 49  | D1    | 23   | THR  | 3.1  |
| 1   | CA    | 1441 | A    | 3.1  |
| 19  | CS    | 16   | LEU  | 3.1  |
| 28  | DG    | 106  | SER  | 3.1  |
| 3   | CC    | 156  | ARG  | 3.1  |
| 22  | DA    | 879  | G    | 3.1  |
| 42  | BU    | 50   | PRO  | 3.1  |
| 27  | DF    | 154  | ILE  | 3.1  |
| 4   | CD    | 24   | GLY  | 3.1  |
| 9   | CI    | 108  | ALA  | 3.1  |
| 39  | DR    | 33   | VAL  | 3.1  |
| 3   | CC    | 85   | GLU  | 3.1  |
| 27  | DF    | 83   | TYR  | 3.1  |
| 43  | DV    | 42   | LEU  | 3.1  |
| 44  | DW    | 53   | CYS  | 3.1  |
| 49  | D1    | 32   | GLU  | 3.1  |
| 30  | DI    | 38   | PHE  | 3.1  |
| 22  | DA    | 2128 | G    | 3.1  |
| 10  | CJ    | 98   | VAL  | 3.1  |
| 27  | DF    | 55   | ALA  | 3.1  |
| 27  | DF    | 82   | GLY  | 3.1  |
| 22  | DA    | 2143 | C    | 3.1  |
| 18  | AR    | 68   | LEU  | 3.1  |
| 26  | DE    | 118  | LEU  | 3.1  |
| 42  | DU    | 43   | LYS  | 3.1  |
| 7   | CG    | 2    | PRO  | 3.1  |
| 1   | CA    | 4    | U    | 3.1  |
| 1   | CA    | 1033 | G    | 3.1  |
| 14  | CN    | 8    | ALA  | 3.1  |
| 30  | BI    | 33   | VAL  | 3.1  |
| 36  | DO    | 14   | ALA  | 3.1  |
| 9   | CI    | 115  | LYS  | 3.1  |
| 23  | DB    | 35   | C    | 3.1  |
| 9   | CI    | 118  | LEU  | 3.1  |
| 3   | AC    | 168  | TYR  | 3.1  |
| 27  | DF    | 7    | TYR  | 3.1  |
| 45  | DX    | 17   | ASN  | 3.1  |
| 51  | D3    | 49   | MET  | 3.1  |
| 20  | CT    | 39   | ILE  | 3.1  |
| 9   | AI    | 41   | ARG  | 3.1  |
| 22  | DA    | 1176 | U    | 3.1  |
| 30  | BI    | 7    | ALA  | 3.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 30  | DI    | 124  | ALA  | 3.1  |
| 43  | DV    | 55   | GLU  | 3.1  |
| 1   | AA    | 1032 | G    | 3.1  |
| 22  | DA    | 1100 | C    | 3.1  |
| 26  | DE    | 200  | LEU  | 3.1  |
| 41  | BT    | 2    | ILE  | 3.1  |
| 13  | CM    | 35   | ALA  | 3.1  |
| 33  | DL    | 83   | ALA  | 3.1  |
| 1   | CA    | 1314 | C    | 3.1  |
| 33  | DL    | 50   | PHE  | 3.1  |
| 4   | AD    | 151  | LYS  | 3.1  |
| 7   | CG    | 38   | THR  | 3.1  |
| 16  | CP    | 17   | TYR  | 3.1  |
| 9   | CI    | 10   | GLY  | 3.1  |
| 10  | CJ    | 33   | GLY  | 3.1  |
| 28  | DG    | 110  | SER  | 3.1  |
| 35  | DN    | 118  | ARG  | 3.1  |
| 38  | DQ    | 37   | GLN  | 3.1  |
| 49  | D1    | 45   | GLN  | 3.1  |
| 14  | CN    | 17   | ALA  | 3.1  |
| 22  | BA    | 1072 | C    | 3.1  |
| 22  | DA    | 2667 | C    | 3.1  |
| 23  | DB    | 118  | C    | 3.1  |
| 9   | CI    | 40   | GLY  | 3.1  |
| 18  | AR    | 23   | TYR  | 3.1  |
| 28  | DG    | 19   | ILE  | 3.1  |
| 45  | DX    | 31   | PRO  | 3.1  |
| 36  | DO    | 50   | ALA  | 3.0  |
| 38  | DQ    | 22   | LYS  | 3.0  |
| 42  | DU    | 26   | LYS  | 3.0  |
| 22  | DA    | 892  | A    | 3.0  |
| 13  | CM    | 88   | GLY  | 3.0  |
| 38  | DQ    | 25   | TYR  | 3.0  |
| 53  | B5    | 21   | TYR  | 3.0  |
| 36  | DO    | 5    | SER  | 3.0  |
| 41  | DT    | 16   | VAL  | 3.0  |
| 9   | CI    | 16   | ALA  | 3.0  |
| 23  | DB    | 21   | G    | 3.0  |
| 30  | DI    | 14   | ALA  | 3.0  |
| 31  | DJ    | 47   | HIS  | 3.0  |
| 53  | B5    | 40   | GLU  | 3.0  |
| 13  | AM    | 27   | LYS  | 3.0  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 14  | CN    | 31   | ILE  | 3.0  |
| 22  | BA    | 1100 | C    | 3.0  |
| 19  | CS    | 79   | THR  | 3.0  |
| 27  | DF    | 146  | VAL  | 3.0  |
| 44  | DW    | 61   | ALA  | 3.0  |
| 9   | CI    | 103  | PHE  | 3.0  |
| 15  | CO    | 17   | ARG  | 3.0  |
| 22  | BA    | 1068 | G    | 3.0  |
| 26  | DE    | 124  | PHE  | 3.0  |
| 27  | DF    | 14   | LYS  | 3.0  |
| 28  | DG    | 53   | GLY  | 3.0  |
| 34  | DM    | 8    | LYS  | 3.0  |
| 2   | CB    | 40   | ILE  | 3.0  |
| 28  | DG    | 74   | SER  | 3.0  |
| 44  | DW    | 85   | GLU  | 3.0  |
| 13  | AM    | 85   | CYS  | 3.0  |
| 22  | DA    | 75   | G    | 3.0  |
| 22  | DA    | 881  | G    | 3.0  |
| 1   | CA    | 1236 | A    | 3.0  |
| 10  | CJ    | 94   | ALA  | 3.0  |
| 27  | DF    | 162  | SER  | 3.0  |
| 28  | DG    | 42   | GLU  | 3.0  |
| 47  | DZ    | 8    | THR  | 3.0  |
| 28  | DG    | 134  | LYS  | 3.0  |
| 36  | DO    | 4    | LYS  | 3.0  |
| 27  | DF    | 119  | ALA  | 3.0  |
| 30  | BI    | 76   | ALA  | 3.0  |
| 35  | DN    | 25   | ALA  | 3.0  |
| 36  | DO    | 88   | LYS  | 3.0  |
| 44  | DW    | 60   | PHE  | 3.0  |
| 41  | DT    | 73   | ARG  | 3.0  |
| 27  | BF    | 42   | GLU  | 3.0  |
| 30  | DI    | 9    | VAL  | 3.0  |
| 7   | CG    | 117  | ALA  | 3.0  |
| 30  | BI    | 62   | TYR  | 3.0  |
| 28  | DG    | 148  | LEU  | 3.0  |
| 35  | DN    | 98   | LEU  | 3.0  |
| 22  | BA    | 1090 | A    | 3.0  |
| 22  | DA    | 2602 | A    | 3.0  |
| 28  | DG    | 44   | LYS  | 3.0  |
| 52  | D4    | 32   | LYS  | 3.0  |
| 26  | DE    | 127  | GLU  | 3.0  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 39  | DR    | 37   | GLU  | 3.0  |
| 48  | D0    | 38   | HIS  | 3.0  |
| 7   | CG    | 65   | ALA  | 3.0  |
| 42  | DU    | 55   | PRO  | 3.0  |
| 22  | DA    | 1534 | U    | 3.0  |
| 29  | BH    | 11   | ASN  | 3.0  |
| 13  | CM    | 3    | ARG  | 3.0  |
| 38  | DQ    | 23   | GLY  | 3.0  |
| 2   | AB    | 128  | LYS  | 3.0  |
| 30  | DI    | 132  | THR  | 3.0  |
| 42  | DU    | 33   | LYS  | 3.0  |
| 53  | B5    | 127  | LYS  | 3.0  |
| 1   | CA    | 1035 | A    | 3.0  |
| 10  | CJ    | 51   | VAL  | 3.0  |
| 1   | AA    | 4    | U    | 2.9  |
| 19  | AS    | 81   | ARG  | 2.9  |
| 22  | BA    | 2585 | U    | 2.9  |
| 25  | DD    | 186  | LEU  | 2.9  |
| 33  | DL    | 114  | GLY  | 2.9  |
| 42  | DU    | 44   | LYS  | 2.9  |
| 43  | DV    | 34   | LYS  | 2.9  |
| 22  | DA    | 2341 | G    | 2.9  |
| 27  | DF    | 68   | THR  | 2.9  |
| 24  | DC    | 172  | VAL  | 2.9  |
| 20  | CT    | 8    | LYS  | 2.9  |
| 22  | DA    | 280  | U    | 2.9  |
| 30  | DI    | 72   | LYS  | 2.9  |
| 51  | D3    | 15   | LYS  | 2.9  |
| 28  | DG    | 30   | ASN  | 2.9  |
| 18  | CR    | 20   | GLU  | 2.9  |
| 37  | DP    | 112  | GLU  | 2.9  |
| 21  | AU    | 42   | THR  | 2.9  |
| 22  | DA    | 1053 | C    | 2.9  |
| 22  | BA    | 883  | G    | 2.9  |
| 22  | DA    | 1091 | G    | 2.9  |
| 23  | DB    | 18   | G    | 2.9  |
| 7   | CG    | 110  | LYS  | 2.9  |
| 21  | CU    | 35   | ARG  | 2.9  |
| 7   | CG    | 150  | ALA  | 2.9  |
| 22  | DA    | 1420 | A    | 2.9  |
| 41  | BT    | 69   | ARG  | 2.9  |
| 20  | AT    | 36   | TYR  | 2.9  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 1          | CA           | 210        | C           | 2.9         |
| 17         | CQ           | 59         | VAL         | 2.9         |
| 40         | DS           | 86         | MET         | 2.9         |
| 20         | CT           | 68         | HIS         | 2.9         |
| 28         | DG           | 133        | LEU         | 2.9         |
| 53         | B5           | 92         | ALA         | 2.9         |
| 30         | BI           | 82         | LYS         | 2.9         |
| 21         | CU           | 47         | ARG         | 2.9         |
| 27         | BF           | 71         | ARG         | 2.9         |
| 9          | AI           | 67         | VAL         | 2.9         |
| 22         | DA           | 2177       | C           | 2.9         |
| 6          | CF           | 8          | PHE         | 2.9         |
| 7          | CG           | 39         | ALA         | 2.9         |
| 11         | CK           | 42         | LEU         | 2.9         |
| 38         | DQ           | 38         | ALA         | 2.9         |
| 22         | DA           | 2111       | U           | 2.9         |
| 22         | DA           | 2796       | U           | 2.9         |
| 53         | B5           | 202        | PRO         | 2.9         |
| 20         | CT           | 85         | LYS         | 2.9         |
| 27         | DF           | 87         | CYS         | 2.9         |
| 33         | DL           | 58         | TYR         | 2.9         |
| 42         | DU           | 54         | GLN         | 2.9         |
| 46         | DY           | 38         | GLN         | 2.9         |
| 30         | BI           | 122        | ILE         | 2.9         |
| 9          | AI           | 128        | SER         | 2.9         |
| 30         | DI           | 71         | THR         | 2.9         |
| 41         | DT           | 53         | VAL         | 2.9         |
| 42         | DU           | 98         | SER         | 2.9         |
| 48         | D0           | 3          | VAL         | 2.9         |
| 27         | DF           | 165        | GLU         | 2.9         |
| 51         | D3           | 26         | HIS         | 2.9         |
| 19         | CS           | 81         | ARG         | 2.9         |
| 30         | BI           | 103        | ARG         | 2.9         |
| 1          | CA           | 1227       | A           | 2.9         |
| 22         | BA           | 1098       | A           | 2.9         |
| 25         | DD           | 26         | VAL         | 2.9         |
| 52         | D4           | 7          | VAL         | 2.9         |
| 3          | CC           | 78         | GLY         | 2.9         |
| 42         | DU           | 31         | SER         | 2.9         |
| 51         | D3           | 53         | GLY         | 2.9         |
| 1          | CA           | 984        | C           | 2.9         |
| 10         | AJ           | 37         | ARG         | 2.9         |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 13  | AM    | 92   | ARG  | 2.9  |
| 22  | BA    | 1061 | U    | 2.9  |
| 22  | BA    | 1926 | U    | 2.9  |
| 14  | CN    | 19   | LYS  | 2.9  |
| 22  | DA    | 1112 | G    | 2.9  |
| 28  | DG    | 6    | LYS  | 2.9  |
| 30  | DI    | 141  | GLU  | 2.9  |
| 7   | CG    | 125  | SER  | 2.9  |
| 11  | AK    | 42   | LEU  | 2.9  |
| 13  | CM    | 113  | ARG  | 2.9  |
| 28  | DG    | 13   | ALA  | 2.9  |
| 28  | DG    | 165  | ALA  | 2.9  |
| 22  | BA    | 140  | C    | 2.9  |
| 19  | CS    | 52   | HIS  | 2.9  |
| 26  | DE    | 165  | HIS  | 2.9  |
| 30  | DI    | 107  | GLN  | 2.9  |
| 13  | CM    | 78   | LYS  | 2.9  |
| 49  | D1    | 5    | ILE  | 2.9  |
| 49  | D1    | 21   | TYR  | 2.9  |
| 9   | AI    | 89   | GLU  | 2.9  |
| 9   | CI    | 31   | ASN  | 2.9  |
| 10  | CJ    | 78   | GLU  | 2.9  |
| 1   | CA    | 1015 | G    | 2.9  |
| 14  | CN    | 16   | LEU  | 2.9  |
| 20  | CT    | 86   | LEU  | 2.9  |
| 22  | DA    | 1056 | G    | 2.9  |
| 24  | DC    | 48   | ARG  | 2.9  |
| 30  | DI    | 137  | GLY  | 2.9  |
| 36  | DO    | 90   | VAL  | 2.9  |
| 28  | DG    | 46   | ALA  | 2.9  |
| 44  | DW    | 63   | ALA  | 2.9  |
| 46  | DY    | 33   | ALA  | 2.9  |
| 33  | DL    | 68   | SER  | 2.8  |
| 29  | DH    | 77   | THR  | 2.8  |
| 26  | DE    | 102  | ARG  | 2.8  |
| 30  | DI    | 16   | GLY  | 2.8  |
| 50  | D2    | 18   | PHE  | 2.8  |
| 22  | DA    | 2860 | A    | 2.8  |
| 42  | DU    | 30   | SER  | 2.8  |
| 1   | CA    | 1126 | U    | 2.8  |
| 12  | AL    | 14   | ARG  | 2.8  |
| 36  | DO    | 114  | GLY  | 2.8  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 19  | AS    | 15   | LEU  | 2.8  |
| 25  | DD    | 132  | ALA  | 2.8  |
| 33  | DL    | 57   | LEU  | 2.8  |
| 22  | DA    | 344  | A    | 2.8  |
| 30  | BI    | 30   | GLN  | 2.8  |
| 22  | BA    | 1729 | U    | 2.8  |
| 1   | CA    | 1214 | C    | 2.8  |
| 22  | DA    | 2630 | G    | 2.8  |
| 32  | DK    | 98   | ARG  | 2.8  |
| 33  | DL    | 117  | THR  | 2.8  |
| 29  | BH    | 145  | ASN  | 2.8  |
| 40  | DS    | 46   | LEU  | 2.8  |
| 3   | CC    | 206  | GLU  | 2.8  |
| 26  | DE    | 55   | SER  | 2.8  |
| 7   | CG    | 26   | PHE  | 2.8  |
| 13  | CM    | 13   | LYS  | 2.8  |
| 14  | AN    | 33   | ASP  | 2.8  |
| 14  | CN    | 7    | LYS  | 2.8  |
| 53  | B5    | 91   | GLY  | 2.8  |
| 7   | AG    | 6    | VAL  | 2.8  |
| 28  | DG    | 132  | VAL  | 2.8  |
| 25  | DD    | 126  | ASN  | 2.8  |
| 26  | DE    | 156  | ASN  | 2.8  |
| 37  | DP    | 97   | LEU  | 2.8  |
| 47  | DZ    | 29   | LEU  | 2.8  |
| 2   | CB    | 133  | GLU  | 2.8  |
| 29  | BH    | 116  | ARG  | 2.8  |
| 1   | CA    | 1286 | U    | 2.8  |
| 11  | AK    | 126  | LYS  | 2.8  |
| 1   | CA    | 1003 | G    | 2.8  |
| 7   | CG    | 90   | GLU  | 2.8  |
| 14  | CN    | 69   | ARG  | 2.8  |
| 19  | AS    | 24   | GLU  | 2.8  |
| 19  | CS    | 65   | GLU  | 2.8  |
| 24  | DC    | 238  | ARG  | 2.8  |
| 25  | DD    | 77   | ARG  | 2.8  |
| 26  | DE    | 190  | ALA  | 2.8  |
| 46  | DY    | 5    | GLU  | 2.8  |
| 1   | CA    | 208  | U    | 2.8  |
| 24  | DC    | 249  | GLY  | 2.8  |
| 26  | DE    | 89   | PRO  | 2.8  |
| 27  | DF    | 44   | ILE  | 2.8  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 45  | DX    | 46   | PHE  | 2.8  |
| 22  | DA    | 2171 | A    | 2.8  |
| 19  | CS    | 3    | ARG  | 2.8  |
| 42  | DU    | 41   | LEU  | 2.8  |
| 25  | DD    | 185  | ASN  | 2.8  |
| 3   | CC    | 195  | VAL  | 2.8  |
| 10  | AJ    | 98   | VAL  | 2.8  |
| 14  | CN    | 53   | ARG  | 2.8  |
| 35  | DN    | 116  | VAL  | 2.8  |
| 14  | AN    | 20   | TYR  | 2.8  |
| 22  | DA    | 2147 | A    | 2.8  |
| 43  | DV    | 6    | ALA  | 2.8  |
| 41  | BT    | 92   | ASN  | 2.8  |
| 1   | AA    | 1026 | G    | 2.8  |
| 5   | CE    | 109  | GLY  | 2.8  |
| 13  | AM    | 47   | GLU  | 2.8  |
| 27  | DF    | 118  | SER  | 2.8  |
| 27  | DF    | 169  | LEU  | 2.8  |
| 51  | D3    | 64   | TYR  | 2.8  |
| 22  | DA    | 405  | U    | 2.7  |
| 2   | CB    | 74   | ARG  | 2.7  |
| 30  | BI    | 59   | ILE  | 2.7  |
| 22  | BA    | 141  | G    | 2.7  |
| 2   | AB    | 57   | LEU  | 2.7  |
| 27  | BF    | 83   | TYR  | 2.7  |
| 47  | DZ    | 2    | ALA  | 2.7  |
| 2   | AB    | 27   | MET  | 2.7  |
| 1   | CA    | 845  | A    | 2.7  |
| 9   | AI    | 4    | ASN  | 2.7  |
| 1   | CA    | 1008 | U    | 2.7  |
| 26  | DE    | 88   | ARG  | 2.7  |
| 3   | CC    | 14   | ILE  | 2.7  |
| 36  | DO    | 80   | GLU  | 2.7  |
| 21  | AU    | 11   | PRO  | 2.7  |
| 19  | AS    | 71   | LEU  | 2.7  |
| 29  | DH    | 75   | LEU  | 2.7  |
| 42  | DU    | 93   | VAL  | 2.7  |
| 45  | DX    | 22   | LEU  | 2.7  |
| 1   | CA    | 1002 | G    | 2.7  |
| 1   | CA    | 1331 | G    | 2.7  |
| 16  | AP    | 82   | ALA  | 2.7  |
| 36  | DO    | 41   | ALA  | 2.7  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 39  | DR    | 28   | ALA  | 2.7  |
| 5   | AE    | 159  | LYS  | 2.7  |
| 34  | DM    | 6    | ARG  | 2.7  |
| 22  | DA    | 544  | C    | 2.7  |
| 2   | AB    | 30   | PHE  | 2.7  |
| 7   | AG    | 18   | PHE  | 2.7  |
| 9   | CI    | 83   | ILE  | 2.7  |
| 4   | CD    | 46   | PRO  | 2.7  |
| 14  | CN    | 33   | ASP  | 2.7  |
| 29  | DH    | 144  | VAL  | 2.7  |
| 32  | DK    | 35   | VAL  | 2.7  |
| 39  | DR    | 20   | VAL  | 2.7  |
| 9   | CI    | 11   | ARG  | 2.7  |
| 21  | AU    | 35   | ARG  | 2.7  |
| 36  | DO    | 107  | ALA  | 2.7  |
| 42  | DU    | 2    | ALA  | 2.7  |
| 43  | DV    | 23   | ALA  | 2.7  |
| 2   | AB    | 65   | GLY  | 2.7  |
| 22  | DA    | 880  | G    | 2.7  |
| 26  | DE    | 150  | THR  | 2.7  |
| 28  | DG    | 25   | THR  | 2.7  |
| 39  | DR    | 19   | THR  | 2.7  |
| 39  | DR    | 31   | GLU  | 2.7  |
| 39  | DR    | 88   | GLY  | 2.7  |
| 46  | DY    | 35   | GLY  | 2.7  |
| 48  | D0    | 23   | THR  | 2.7  |
| 1   | AA    | 1001 | C    | 2.7  |
| 1   | CA    | 1321 | U    | 2.7  |
| 11  | AK    | 113  | VAL  | 2.7  |
| 19  | CS    | 21   | LYS  | 2.7  |
| 28  | DG    | 50   | LEU  | 2.7  |
| 26  | DE    | 10   | SER  | 2.7  |
| 27  | DF    | 107  | ALA  | 2.7  |
| 7   | CG    | 112  | GLY  | 2.7  |
| 9   | CI    | 30   | ILE  | 2.7  |
| 22  | BA    | 879  | G    | 2.7  |
| 27  | DF    | 100  | PHE  | 2.7  |
| 22  | DA    | 2313 | C    | 2.7  |
| 1   | CA    | 81   | A    | 2.7  |
| 19  | CS    | 32   | ARG  | 2.7  |
| 19  | CS    | 58   | VAL  | 2.7  |
| 53  | B5    | 44   | VAL  | 2.7  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 13  | CM    | 5    | ALA  | 2.7  |
| 53  | B5    | 177  | GLY  | 2.7  |
| 6   | CF    | 35   | LYS  | 2.7  |
| 41  | DT    | 30   | ILE  | 2.7  |
| 41  | DT    | 40   | LYS  | 2.7  |
| 26  | DE    | 178  | VAL  | 2.7  |
| 42  | DU    | 25   | VAL  | 2.7  |
| 29  | BH    | 89   | LYS  | 2.7  |
| 27  | BF    | 77   | PHE  | 2.7  |
| 22  | DA    | 102  | U    | 2.7  |
| 26  | DE    | 24   | ASN  | 2.7  |
| 53  | B5    | 189  | ASN  | 2.7  |
| 9   | AI    | 63   | LEU  | 2.7  |
| 17  | CQ    | 63   | GLU  | 2.7  |
| 29  | DH    | 122  | LEU  | 2.7  |
| 33  | DL    | 115  | GLU  | 2.7  |
| 42  | DU    | 81   | ASP  | 2.7  |
| 22  | DA    | 1321 | A    | 2.7  |
| 29  | BH    | 25   | TYR  | 2.7  |
| 7   | CG    | 60   | GLU  | 2.7  |
| 7   | AG    | 69   | VAL  | 2.7  |
| 16  | CP    | 54   | LEU  | 2.7  |
| 1   | CA    | 1001 | C    | 2.7  |
| 30  | BI    | 27   | ALA  | 2.7  |
| 51  | D3    | 27   | ALA  | 2.7  |
| 19  | AS    | 61   | PHE  | 2.6  |
| 29  | DH    | 91   | PHE  | 2.6  |
| 18  | CR    | 51   | TYR  | 2.6  |
| 22  | BA    | 2192 | U    | 2.6  |
| 28  | DG    | 24   | ILE  | 2.6  |
| 3   | CC    | 157  | LEU  | 2.6  |
| 49  | D1    | 43   | VAL  | 2.6  |
| 27  | BF    | 41   | GLY  | 2.6  |
| 22  | DA    | 893  | C    | 2.6  |
| 27  | DF    | 109  | PRO  | 2.6  |
| 27  | DF    | 75   | ALA  | 2.6  |
| 30  | DI    | 103  | ARG  | 2.6  |
| 37  | DP    | 95   | ALA  | 2.6  |
| 2   | CB    | 15   | HIS  | 2.6  |
| 9   | AI    | 83   | ILE  | 2.6  |
| 13  | AM    | 17   | ILE  | 2.6  |
| 22  | DA    | 88   | G    | 2.6  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 22  | DA    | 141  | G    | 2.6  |
| 22  | DA    | 1059 | G    | 2.6  |
| 29  | BH    | 99   | ILE  | 2.6  |
| 30  | BI    | 86   | ILE  | 2.6  |
| 34  | DM    | 62   | LYS  | 2.6  |
| 35  | DN    | 97   | ILE  | 2.6  |
| 2   | AB    | 117  | LEU  | 2.6  |
| 28  | DG    | 117  | LEU  | 2.6  |
| 39  | DR    | 22   | LEU  | 2.6  |
| 46  | DY    | 45   | GLN  | 2.6  |
| 44  | DW    | 64   | ASP  | 2.6  |
| 2   | CB    | 149  | GLY  | 2.6  |
| 10  | AJ    | 38   | GLY  | 2.6  |
| 11  | AK    | 43   | GLY  | 2.6  |
| 26  | DE    | 13   | THR  | 2.6  |
| 7   | AG    | 88   | PRO  | 2.6  |
| 28  | DG    | 35   | ARG  | 2.6  |
| 1   | CA    | 1132 | C    | 2.6  |
| 7   | CG    | 74   | GLU  | 2.6  |
| 27  | DF    | 85   | ILE  | 2.6  |
| 28  | DG    | 131  | ILE  | 2.6  |
| 29  | DH    | 143  | ILE  | 2.6  |
| 31  | DJ    | 118  | MET  | 2.6  |
| 39  | DR    | 49   | ILE  | 2.6  |
| 40  | DS    | 4    | ILE  | 2.6  |
| 28  | DG    | 164  | TYR  | 2.6  |
| 1   | AA    | 412  | A    | 2.6  |
| 1   | AA    | 1042 | A    | 2.6  |
| 2   | AB    | 35   | ARG  | 2.6  |
| 2   | AB    | 187  | VAL  | 2.6  |
| 7   | CG    | 82   | GLY  | 2.6  |
| 14  | AN    | 18   | ASP  | 2.6  |
| 19  | CS    | 62   | VAL  | 2.6  |
| 30  | BI    | 24   | VAL  | 2.6  |
| 35  | DN    | 73   | ASN  | 2.6  |
| 30  | BI    | 73   | THR  | 2.6  |
| 20  | CT    | 47   | ALA  | 2.6  |
| 25  | DD    | 41   | ALA  | 2.6  |
| 46  | DY    | 60   | LYS  | 2.6  |
| 1   | CA    | 1237 | C    | 2.6  |
| 22  | BA    | 2129 | C    | 2.6  |
| 27  | DF    | 42   | GLU  | 2.6  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 8   | CH    | 3    | MET  | 2.6  |
| 33  | DL    | 73   | ILE  | 2.6  |
| 40  | DS    | 103  | ILE  | 2.6  |
| 10  | AJ    | 71   | LEU  | 2.6  |
| 33  | DL    | 7    | SER  | 2.6  |
| 41  | DT    | 50   | LEU  | 2.6  |
| 52  | B4    | 12   | ARG  | 2.6  |
| 2   | AB    | 123  | ASP  | 2.6  |
| 18  | CR    | 40   | VAL  | 2.6  |
| 1   | CA    | 1036 | A    | 2.6  |
| 7   | CG    | 71   | PRO  | 2.6  |
| 30  | BI    | 63   | ALA  | 2.6  |
| 36  | DO    | 57   | ALA  | 2.6  |
| 2   | CB    | 30   | PHE  | 2.6  |
| 1   | CA    | 85   | U    | 2.6  |
| 9   | CI    | 57   | MET  | 2.6  |
| 22  | DA    | 1468 | U    | 2.6  |
| 8   | CH    | 90   | ASP  | 2.6  |
| 17  | CQ    | 83   | VAL  | 2.6  |
| 41  | DT    | 80   | TRP  | 2.6  |
| 41  | DT    | 45   | ALA  | 2.6  |
| 51  | D3    | 65   | ALA  | 2.6  |
| 52  | D4    | 13   | ASN  | 2.6  |
| 1   | CA    | 1275 | A    | 2.6  |
| 2   | CB    | 91   | PHE  | 2.6  |
| 14  | CN    | 21   | PHE  | 2.6  |
| 22  | BA    | 2193 | G    | 2.6  |
| 22  | DA    | 2158 | A    | 2.6  |
| 7   | CG    | 144  | MET  | 2.6  |
| 38  | DQ    | 44   | GLN  | 2.6  |
| 53  | B5    | 19   | LYS  | 2.6  |
| 2   | CB    | 217  | VAL  | 2.6  |
| 10  | CJ    | 91   | ASP  | 2.6  |
| 13  | CM    | 18   | ALA  | 2.6  |
| 10  | CJ    | 37   | ARG  | 2.6  |
| 37  | DP    | 109  | ARG  | 2.6  |
| 44  | DW    | 43   | THR  | 2.6  |
| 12  | CL    | 123  | LYS  | 2.6  |
| 22  | DA    | 291  | G    | 2.6  |
| 25  | DD    | 96   | ILE  | 2.6  |
| 22  | DA    | 1101 | U    | 2.6  |
| 30  | BI    | 9    | VAL  | 2.6  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 30  | DI    | 116  | ASP  | 2.6  |
| 29  | BH    | 81   | ALA  | 2.6  |
| 29  | DH    | 84   | ALA  | 2.6  |
| 46  | DY    | 48   | ARG  | 2.6  |
| 2   | AB    | 67   | ILE  | 2.6  |
| 1   | CA    | 978  | A    | 2.6  |
| 10  | CJ    | 15   | HIS  | 2.6  |
| 26  | DE    | 199  | MET  | 2.6  |
| 22  | DA    | 1092 | C    | 2.6  |
| 22  | DA    | 1408 | G    | 2.6  |
| 39  | DR    | 34   | GLU  | 2.6  |
| 41  | DT    | 56   | GLU  | 2.6  |
| 13  | AM    | 35   | ALA  | 2.6  |
| 29  | DH    | 47   | PHE  | 2.6  |
| 40  | DS    | 93   | ALA  | 2.6  |
| 2   | AB    | 129  | LEU  | 2.5  |
| 3   | CC    | 107  | ARG  | 2.5  |
| 36  | DO    | 9    | ARG  | 2.5  |
| 13  | CM    | 112  | PRO  | 2.5  |
| 41  | DT    | 89   | GLU  | 2.5  |
| 27  | DF    | 47   | LYS  | 2.5  |
| 36  | DO    | 81   | ARG  | 2.5  |
| 40  | DS    | 6    | LYS  | 2.5  |
| 33  | DL    | 85   | VAL  | 2.5  |
| 46  | DY    | 47   | ARG  | 2.5  |
| 1   | CA    | 1209 | C    | 2.5  |
| 22  | DA    | 1533 | C    | 2.5  |
| 1   | CA    | 1270 | G    | 2.5  |
| 20  | CT    | 45   | ALA  | 2.5  |
| 29  | DH    | 10   | ALA  | 2.5  |
| 37  | DP    | 19   | SER  | 2.5  |
| 2   | AB    | 29   | PRO  | 2.5  |
| 25  | DD    | 76   | GLY  | 2.5  |
| 35  | DN    | 26   | GLY  | 2.5  |
| 35  | DN    | 93   | GLY  | 2.5  |
| 43  | DV    | 89   | ILE  | 2.5  |
| 46  | BY    | 2    | LYS  | 2.5  |
| 46  | DY    | 62   | GLY  | 2.5  |
| 13  | CM    | 93   | ARG  | 2.5  |
| 29  | BH    | 5    | LEU  | 2.5  |
| 41  | DT    | 77   | ARG  | 2.5  |
| 13  | CM    | 28   | THR  | 2.5  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | CA    | 1218 | C    | 2.5  |
| 2   | CB    | 182  | PRO  | 2.5  |
| 29  | DH    | 137  | GLU  | 2.5  |
| 10  | CJ    | 40   | ILE  | 2.5  |
| 23  | DB    | 20   | G    | 2.5  |
| 35  | DN    | 107  | ASN  | 2.5  |
| 38  | DQ    | 82   | GLY  | 2.5  |
| 43  | DV    | 49   | ASN  | 2.5  |
| 2   | CB    | 107  | VAL  | 2.5  |
| 9   | AI    | 48   | VAL  | 2.5  |
| 22  | DA    | 646  | U    | 2.5  |
| 29  | BH    | 138  | VAL  | 2.5  |
| 30  | BI    | 139  | VAL  | 2.5  |
| 43  | DV    | 1    | MET  | 2.5  |
| 9   | CI    | 91   | ASP  | 2.5  |
| 19  | CS    | 77   | THR  | 2.5  |
| 12  | CL    | 44   | LYS  | 2.5  |
| 27  | DF    | 171  | ALA  | 2.5  |
| 36  | DO    | 30   | ARG  | 2.5  |
| 52  | D4    | 38   | GLY  | 2.5  |
| 10  | CJ    | 6    | ILE  | 2.5  |
| 25  | DD    | 27   | ILE  | 2.5  |
| 39  | DR    | 101  | ILE  | 2.5  |
| 1   | AA    | 842  | U    | 2.5  |
| 22  | BA    | 880  | G    | 2.5  |
| 23  | DB    | 64   | G    | 2.5  |
| 6   | CF    | 80   | PHE  | 2.5  |
| 7   | AG    | 151  | PHE  | 2.5  |
| 41  | DT    | 49   | LYS  | 2.5  |
| 51  | D3    | 24   | HIS  | 2.5  |
| 14  | CN    | 99   | ALA  | 2.5  |
| 38  | DQ    | 30   | ARG  | 2.5  |
| 42  | DU    | 75   | ALA  | 2.5  |
| 52  | D4    | 36   | ARG  | 2.5  |
| 51  | D3    | 59   | ILE  | 2.5  |
| 13  | AM    | 105  | ASN  | 2.5  |
| 25  | DD    | 56   | LYS  | 2.5  |
| 29  | DH    | 57   | LYS  | 2.5  |
| 2   | AB    | 18   | HIS  | 2.5  |
| 29  | BH    | 76   | GLU  | 2.5  |
| 39  | DR    | 103  | ALA  | 2.5  |
| 20  | CT    | 13   | GLN  | 2.5  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 5   | AE    | 115  | LEU  | 2.5  |
| 17  | CQ    | 44   | LEU  | 2.5  |
| 27  | DF    | 9    | LYS  | 2.5  |
| 30  | BI    | 106  | LEU  | 2.5  |
| 39  | DR    | 24   | LYS  | 2.5  |
| 46  | BY    | 6    | LEU  | 2.5  |
| 14  | CN    | 43   | ASN  | 2.5  |
| 30  | BI    | 43   | ASN  | 2.5  |
| 14  | CN    | 6    | MET  | 2.5  |
| 15  | CO    | 26   | GLU  | 2.5  |
| 20  | CT    | 43   | ASP  | 2.5  |
| 46  | DY    | 26   | PHE  | 2.5  |
| 22  | DA    | 548  | G    | 2.5  |
| 25  | DD    | 209  | ALA  | 2.5  |
| 34  | DM    | 29   | GLY  | 2.5  |
| 46  | DY    | 3    | ALA  | 2.5  |
| 13  | CM    | 110  | LYS  | 2.5  |
| 1   | CA    | 841  | C    | 2.5  |
| 2   | CB    | 161  | LEU  | 2.5  |
| 17  | CQ    | 75   | LEU  | 2.5  |
| 22  | DA    | 2129 | C    | 2.5  |
| 33  | DL    | 107  | PHE  | 2.5  |
| 2   | CB    | 128  | LYS  | 2.5  |
| 11  | AK    | 19   | GLY  | 2.5  |
| 20  | AT    | 64   | LYS  | 2.5  |
| 27  | DF    | 81   | GLN  | 2.5  |
| 1   | CA    | 1455 | G    | 2.5  |
| 6   | AF    | 54   | LEU  | 2.5  |
| 9   | AI    | 6    | TYR  | 2.5  |
| 18  | AR    | 32   | TYR  | 2.5  |
| 22  | DA    | 2801 | G    | 2.5  |
| 24  | DC    | 205  | LEU  | 2.5  |
| 6   | CF    | 91   | ARG  | 2.4  |
| 14  | CN    | 63   | ARG  | 2.4  |
| 22  | DA    | 33   | C    | 2.4  |
| 22  | DA    | 436  | C    | 2.4  |
| 26  | DE    | 179  | SER  | 2.4  |
| 52  | D4    | 30   | GLU  | 2.4  |
| 46  | DY    | 1    | MET  | 2.4  |
| 1   | CA    | 1492 | A    | 2.4  |
| 22  | DA    | 1205 | A    | 2.4  |
| 36  | DO    | 3    | LYS  | 2.4  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 42  | DU    | 91   | LYS  | 2.4  |
| 29  | BH    | 126  | GLY  | 2.4  |
| 42  | BU    | 57   | GLY  | 2.4  |
| 2   | AB    | 15   | HIS  | 2.4  |
| 48  | D0    | 2    | ALA  | 2.4  |
| 7   | CG    | 44   | TYR  | 2.4  |
| 10  | CJ    | 31   | ARG  | 2.4  |
| 17  | CQ    | 61   | ILE  | 2.4  |
| 29  | DH    | 72   | ILE  | 2.4  |
| 30  | DI    | 37   | GLU  | 2.4  |
| 1   | CA    | 987  | G    | 2.4  |
| 14  | CN    | 55   | SER  | 2.4  |
| 46  | DY    | 40   | SER  | 2.4  |
| 1   | CA    | 995  | C    | 2.4  |
| 22  | DA    | 897  | C    | 2.4  |
| 23  | DB    | 19   | C    | 2.4  |
| 24  | DC    | 26   | LYS  | 2.4  |
| 39  | DR    | 1    | MET  | 2.4  |
| 46  | DY    | 9    | LYS  | 2.4  |
| 43  | DV    | 43   | ASP  | 2.4  |
| 21  | AU    | 50   | ALA  | 2.4  |
| 28  | DG    | 174  | ALA  | 2.4  |
| 33  | DL    | 15   | ALA  | 2.4  |
| 1   | CA    | 80   | A    | 2.4  |
| 22  | DA    | 2211 | A    | 2.4  |
| 2   | CB    | 137  | ARG  | 2.4  |
| 3   | CC    | 126  | ARG  | 2.4  |
| 17  | CQ    | 77   | ARG  | 2.4  |
| 49  | D1    | 46   | HIS  | 2.4  |
| 14  | CN    | 46   | LEU  | 2.4  |
| 41  | DT    | 54   | GLU  | 2.4  |
| 42  | DU    | 15   | THR  | 2.4  |
| 2   | AB    | 213  | TYR  | 2.4  |
| 3   | AC    | 193  | TYR  | 2.4  |
| 20  | CT    | 36   | TYR  | 2.4  |
| 4   | AD    | 177  | LYS  | 2.4  |
| 24  | DC    | 5    | LYS  | 2.4  |
| 30  | DI    | 113  | LYS  | 2.4  |
| 22  | DA    | 316  | C    | 2.4  |
| 36  | DO    | 105  | ALA  | 2.4  |
| 3   | CC    | 162  | ILE  | 2.4  |
| 10  | AJ    | 25   | ILE  | 2.4  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 22  | DA    | 1509 | A    | 2.4  |
| 45  | DX    | 30   | LEU  | 2.4  |
| 40  | DS    | 100  | THR  | 2.4  |
| 3   | CC    | 37   | PHE  | 2.4  |
| 6   | AF    | 89   | VAL  | 2.4  |
| 33  | DL    | 122  | VAL  | 2.4  |
| 7   | CG    | 81   | GLY  | 2.4  |
| 26  | DE    | 1    | MET  | 2.4  |
| 35  | DN    | 62   | ASN  | 2.4  |
| 6   | CF    | 79   | ARG  | 2.4  |
| 36  | DO    | 19   | GLN  | 2.4  |
| 38  | DQ    | 59   | GLN  | 2.4  |
| 8   | CH    | 130  | ALA  | 2.4  |
| 27  | DF    | 168  | ALA  | 2.4  |
| 22  | DA    | 1214 | A    | 2.4  |
| 27  | DF    | 132  | VAL  | 2.4  |
| 34  | DM    | 64   | TRP  | 2.4  |
| 21  | AU    | 24   | GLU  | 2.4  |
| 36  | DO    | 38   | GLN  | 2.4  |
| 42  | BU    | 46   | GLN  | 2.4  |
| 53  | B5    | 168  | LYS  | 2.4  |
| 36  | DO    | 23   | ALA  | 2.4  |
| 53  | B5    | 159  | ALA  | 2.4  |
| 1   | CA    | 460  | A    | 2.4  |
| 10  | CJ    | 32   | THR  | 2.4  |
| 11  | AK    | 13   | ARG  | 2.4  |
| 27  | DF    | 71   | ARG  | 2.4  |
| 28  | DG    | 171  | THR  | 2.4  |
| 30  | BI    | 93   | PRO  | 2.4  |
| 30  | DI    | 26   | PRO  | 2.4  |
| 31  | DJ    | 74   | TYR  | 2.4  |
| 7   | AG    | 56   | LYS  | 2.4  |
| 22  | DA    | 508  | A    | 2.4  |
| 41  | DT    | 86   | THR  | 2.4  |
| 26  | DE    | 9    | GLN  | 2.4  |
| 27  | BF    | 81   | GLN  | 2.4  |
| 29  | BH    | 20   | ASN  | 2.4  |
| 34  | DM    | 27   | SER  | 2.4  |
| 43  | DV    | 45   | ASP  | 2.4  |
| 3   | CC    | 102  | ASN  | 2.4  |
| 10  | AJ    | 34   | ALA  | 2.4  |
| 21  | AU    | 52   | ALA  | 2.4  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 29  | BH    | 111  | ALA  | 2.4  |
| 3   | CC    | 87   | LEU  | 2.4  |
| 36  | DO    | 87   | ILE  | 2.4  |
| 35  | DN    | 30   | ARG  | 2.4  |
| 27  | DF    | 74   | VAL  | 2.4  |
| 33  | DL    | 118  | THR  | 2.4  |
| 22  | BA    | 1089 | A    | 2.4  |
| 3   | CC    | 141  | ALA  | 2.4  |
| 22  | DA    | 228  | C    | 2.4  |
| 29  | BH    | 4    | ILE  | 2.4  |
| 27  | DF    | 30   | ARG  | 2.4  |
| 7   | CG    | 6    | VAL  | 2.4  |
| 24  | DC    | 245  | VAL  | 2.4  |
| 28  | DG    | 169  | VAL  | 2.4  |
| 42  | DU    | 83   | VAL  | 2.4  |
| 13  | CM    | 82   | ASP  | 2.4  |
| 1   | CA    | 1362 | A    | 2.4  |
| 13  | CM    | 15   | ALA  | 2.4  |
| 22  | DA    | 1111 | A    | 2.4  |
| 22  | DA    | 1169 | A    | 2.4  |
| 34  | DM    | 56   | ALA  | 2.4  |
| 46  | DY    | 32   | ALA  | 2.4  |
| 10  | AJ    | 90   | LEU  | 2.4  |
| 13  | CM    | 57   | ARG  | 2.4  |
| 32  | DK    | 53   | LYS  | 2.4  |
| 41  | DT    | 69   | ARG  | 2.4  |
| 22  | DA    | 2164 | C    | 2.4  |
| 27  | DF    | 99   | PHE  | 2.3  |
| 28  | DG    | 31   | GLY  | 2.3  |
| 41  | DT    | 10   | VAL  | 2.3  |
| 1   | CA    | 467  | U    | 2.3  |
| 1   | CA    | 1224 | U    | 2.3  |
| 1   | CA    | 1307 | U    | 2.3  |
| 2   | CB    | 88   | ASP  | 2.3  |
| 22  | DA    | 2105 | U    | 2.3  |
| 37  | DP    | 13   | MET  | 2.3  |
| 20  | CT    | 87   | ALA  | 2.3  |
| 22  | DA    | 619  | G    | 2.3  |
| 22  | DA    | 1212 | G    | 2.3  |
| 29  | BH    | 65   | ALA  | 2.3  |
| 28  | DG    | 38   | ASN  | 2.3  |
| 49  | D1    | 44   | ARG  | 2.3  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 48         | D0           | 39         | LEU         | 2.3         |
| 22         | BA           | 893        | C           | 2.3         |
| 22         | DA           | 2178       | C           | 2.3         |
| 28         | DG           | 28         | GLY         | 2.3         |
| 33         | DL           | 124        | GLY         | 2.3         |
| 22         | DA           | 2149       | U           | 2.3         |
| 38         | DQ           | 45         | TYR         | 2.3         |
| 7          | CG           | 115        | SER         | 2.3         |
| 26         | DE           | 180        | LEU         | 2.3         |
| 22         | BA           | 1062       | G           | 2.3         |
| 22         | DA           | 583        | G           | 2.3         |
| 22         | DA           | 1734       | G           | 2.3         |
| 37         | BP           | 115        | ASN         | 2.3         |
| 40         | DS           | 40         | ASN         | 2.3         |
| 43         | DV           | 58         | SER         | 2.3         |
| 51         | D3           | 28         | ASN         | 2.3         |
| 1          | CA           | 1493       | A           | 2.3         |
| 25         | DD           | 6          | GLY         | 2.3         |
| 27         | DF           | 138        | PHE         | 2.3         |
| 53         | B5           | 209        | PHE         | 2.3         |
| 26         | DE           | 90         | GLN         | 2.3         |
| 26         | DE           | 96         | VAL         | 2.3         |
| 28         | DG           | 4          | VAL         | 2.3         |
| 41         | DT           | 31         | VAL         | 2.3         |
| 1          | CA           | 842        | U           | 2.3         |
| 22         | DA           | 2182       | U           | 2.3         |
| 28         | DG           | 137        | ASP         | 2.3         |
| 30         | BI           | 47         | ASP         | 2.3         |
| 41         | DT           | 46         | ALA         | 2.3         |
| 7          | CG           | 129        | GLU         | 2.3         |
| 14         | AN           | 26         | GLU         | 2.3         |
| 29         | DH           | 149        | GLU         | 2.3         |
| 30         | BI           | 112        | THR         | 2.3         |
| 33         | DL           | 5          | THR         | 2.3         |
| 33         | DL           | 77         | ILE         | 2.3         |
| 37         | DP           | 114        | LEU         | 2.3         |
| 51         | D3           | 6          | THR         | 2.3         |
| 21         | AU           | 51         | SER         | 2.3         |
| 9          | AI           | 39         | PHE         | 2.3         |
| 44         | DW           | 73         | GLY         | 2.3         |
| 15         | CO           | 75         | VAL         | 2.3         |
| 22         | DA           | 279        | A           | 2.3         |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 27  | DF    | 115  | ARG  | 2.3  |
| 30  | BI    | 65   | ARG  | 2.3  |
| 39  | DR    | 51   | VAL  | 2.3  |
| 22  | DA    | 1730 | C    | 2.3  |
| 22  | DA    | 2798 | U    | 2.3  |
| 36  | DO    | 108  | ASP  | 2.3  |
| 45  | DX    | 78   | TYR  | 2.3  |
| 49  | D1    | 35   | GLU  | 2.3  |
| 4   | AD    | 82   | LEU  | 2.3  |
| 20  | CT    | 79   | LEU  | 2.3  |
| 27  | DF    | 57   | LEU  | 2.3  |
| 28  | DG    | 36   | THR  | 2.3  |
| 14  | CN    | 68   | GLY  | 2.3  |
| 24  | BC    | 237  | GLY  | 2.3  |
| 25  | DD    | 125  | TRP  | 2.3  |
| 50  | D2    | 30   | VAL  | 2.3  |
| 1   | CA    | 1241 | G    | 2.3  |
| 1   | CA    | 1287 | A    | 2.3  |
| 22  | DA    | 1538 | G    | 2.3  |
| 1   | CA    | 1212 | U    | 2.3  |
| 14  | CN    | 3    | LYS  | 2.3  |
| 28  | BG    | 177  | LYS  | 2.3  |
| 2   | AB    | 20   | THR  | 2.3  |
| 7   | AG    | 78   | ARG  | 2.3  |
| 14  | CN    | 41   | ARG  | 2.3  |
| 33  | DL    | 26   | GLY  | 2.3  |
| 39  | DR    | 35   | PHE  | 2.3  |
| 7   | CG    | 20   | SER  | 2.3  |
| 45  | DX    | 20   | HIS  | 2.3  |
| 22  | DA    | 549  | G    | 2.3  |
| 22  | DA    | 603  | A    | 2.3  |
| 22  | DA    | 1052 | C    | 2.3  |
| 29  | DH    | 86   | ASP  | 2.3  |
| 22  | DA    | 2108 | A    | 2.3  |
| 22  | DA    | 2412 | A    | 2.3  |
| 29  | BH    | 26   | ALA  | 2.3  |
| 36  | DO    | 25   | ARG  | 2.3  |
| 19  | AS    | 41   | PHE  | 2.3  |
| 29  | DH    | 132  | PHE  | 2.3  |
| 28  | DG    | 88   | GLN  | 2.3  |
| 2   | CB    | 210  | VAL  | 2.3  |
| 30  | BI    | 102  | SER  | 2.3  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 10  | CJ    | 11   | LYS  | 2.3  |
| 28  | DG    | 12   | PRO  | 2.3  |
| 31  | DJ    | 97   | PRO  | 2.3  |
| 1   | CA    | 1325 | C    | 2.3  |
| 30  | BI    | 36   | MET  | 2.3  |
| 34  | DM    | 105  | MET  | 2.3  |
| 3   | CC    | 159  | GLY  | 2.3  |
| 9   | AI    | 28   | ILE  | 2.3  |
| 18  | AR    | 21   | ILE  | 2.3  |
| 2   | AB    | 32   | PHE  | 2.3  |
| 15  | CO    | 15   | PHE  | 2.3  |
| 22  | DA    | 1042 | G    | 2.3  |
| 25  | DD    | 115  | GLY  | 2.3  |
| 31  | DJ    | 119  | PHE  | 2.3  |
| 43  | DV    | 91   | PHE  | 2.3  |
| 25  | DD    | 49   | GLN  | 2.3  |
| 13  | AM    | 43   | VAL  | 2.3  |
| 27  | DF    | 121  | SER  | 2.3  |
| 42  | DU    | 37   | GLU  | 2.3  |
| 2   | AB    | 127  | ASP  | 2.3  |
| 13  | AM    | 109  | ARG  | 2.3  |
| 22  | DA    | 1542 | U    | 2.3  |
| 25  | DD    | 84   | LEU  | 2.3  |
| 1   | AA    | 1027 | C    | 2.3  |
| 13  | CM    | 81   | MET  | 2.3  |
| 20  | CT    | 67   | ILE  | 2.3  |
| 35  | DN    | 94   | TYR  | 2.3  |
| 35  | DN    | 113  | ILE  | 2.3  |
| 7   | AG    | 58   | GLU  | 2.3  |
| 10  | CJ    | 66   | GLU  | 2.3  |
| 13  | CM    | 41   | GLU  | 2.3  |
| 23  | DB    | 16   | G    | 2.3  |
| 35  | DN    | 82   | GLU  | 2.3  |
| 28  | DG    | 127  | THR  | 2.2  |
| 3   | CC    | 179  | ARG  | 2.2  |
| 46  | DY    | 29   | ARG  | 2.2  |
| 14  | CN    | 18   | ASP  | 2.2  |
| 22  | DA    | 1217 | U    | 2.2  |
| 44  | DW    | 57   | HIS  | 2.2  |
| 10  | CJ    | 38   | GLY  | 2.2  |
| 53  | B5    | 201  | LYS  | 2.2  |
| 36  | DO    | 84   | GLU  | 2.2  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | CA    | 101  | A    | 2.2  |
| 22  | BA    | 1088 | A    | 2.2  |
| 22  | DA    | 1872 | A    | 2.2  |
| 20  | CT    | 70   | ASN  | 2.2  |
| 36  | DO    | 54   | VAL  | 2.2  |
| 1   | CA    | 1050 | G    | 2.2  |
| 2   | CB    | 116  | ASP  | 2.2  |
| 2   | CB    | 159  | ASP  | 2.2  |
| 2   | CB    | 39   | HIS  | 2.2  |
| 3   | AC    | 86   | LYS  | 2.2  |
| 48  | D0    | 53   | LYS  | 2.2  |
| 7   | CG    | 121  | ALA  | 2.2  |
| 13  | AM    | 99   | GLY  | 2.2  |
| 19  | AS    | 13   | LEU  | 2.2  |
| 19  | CS    | 46   | GLY  | 2.2  |
| 33  | DL    | 102  | GLY  | 2.2  |
| 40  | DS    | 5    | ALA  | 2.2  |
| 41  | DT    | 32   | LEU  | 2.2  |
| 43  | DV    | 33   | GLY  | 2.2  |
| 28  | DG    | 141  | ILE  | 2.2  |
| 31  | DJ    | 142  | ILE  | 2.2  |
| 19  | CS    | 73   | GLU  | 2.2  |
| 21  | AU    | 10   | GLU  | 2.2  |
| 33  | DL    | 86   | GLU  | 2.2  |
| 48  | D0    | 49   | TYR  | 2.2  |
| 9   | CI    | 67   | VAL  | 2.2  |
| 19  | AS    | 60   | VAL  | 2.2  |
| 28  | DG    | 149  | ARG  | 2.2  |
| 29  | DH    | 110  | VAL  | 2.2  |
| 2   | AB    | 66   | LYS  | 2.2  |
| 41  | DT    | 36   | LYS  | 2.2  |
| 10  | CJ    | 44   | THR  | 2.2  |
| 22  | BA    | 882  | G    | 2.2  |
| 22  | DA    | 1475 | G    | 2.2  |
| 23  | DB    | 2    | G    | 2.2  |
| 27  | DF    | 116  | GLY  | 2.2  |
| 38  | DQ    | 73   | GLY  | 2.2  |
| 20  | CT    | 12   | ILE  | 2.2  |
| 18  | CR    | 73   | ARG  | 2.2  |
| 28  | DG    | 157  | TYR  | 2.2  |
| 39  | DR    | 92   | TRP  | 2.2  |
| 22  | DA    | 2146 | C    | 2.2  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 5   | CE    | 149  | SER  | 2.2  |
| 6   | AF    | 61   | LEU  | 2.2  |
| 7   | CG    | 30   | LEU  | 2.2  |
| 10  | CJ    | 24   | GLU  | 2.2  |
| 53  | B5    | 190  | ILE  | 2.2  |
| 10  | AJ    | 7    | ARG  | 2.2  |
| 10  | AJ    | 89   | ARG  | 2.2  |
| 22  | DA    | 2162 | G    | 2.2  |
| 42  | DU    | 22   | ARG  | 2.2  |
| 29  | BH    | 147  | VAL  | 2.2  |
| 29  | DH    | 78   | VAL  | 2.2  |
| 22  | DA    | 1060 | U    | 2.2  |
| 1   | CA    | 1363 | A    | 2.2  |
| 5   | CE    | 124  | LEU  | 2.2  |
| 4   | CD    | 47   | ARG  | 2.2  |
| 7   | AG    | 79   | ARG  | 2.2  |
| 22  | DA    | 2799 | A    | 2.2  |
| 26  | DE    | 157  | LEU  | 2.2  |
| 25  | DD    | 47   | ALA  | 2.2  |
| 27  | DF    | 20   | PHE  | 2.2  |
| 36  | DO    | 13   | ARG  | 2.2  |
| 36  | DO    | 53   | THR  | 2.2  |
| 50  | D2    | 14   | ARG  | 2.2  |
| 28  | DG    | 22   | GLN  | 2.2  |
| 28  | DG    | 29   | LYS  | 2.2  |
| 46  | DY    | 25   | GLN  | 2.2  |
| 13  | CM    | 99   | GLY  | 2.2  |
| 19  | AS    | 20   | GLU  | 2.2  |
| 33  | DL    | 130  | GLY  | 2.2  |
| 2   | AB    | 42   | ASN  | 2.2  |
| 13  | CM    | 42   | ASP  | 2.2  |
| 3   | AC    | 64   | ILE  | 2.2  |
| 6   | AF    | 6    | ILE  | 2.2  |
| 11  | AK    | 110  | ILE  | 2.2  |
| 14  | CN    | 73   | PHE  | 2.2  |
| 19  | CS    | 10   | PHE  | 2.2  |
| 22  | DA    | 1061 | U    | 2.2  |
| 25  | DD    | 201  | LEU  | 2.2  |
| 26  | DE    | 183  | PHE  | 2.2  |
| 28  | DG    | 129  | THR  | 2.2  |
| 1   | CA    | 1219 | A    | 2.2  |
| 3   | AC    | 66   | VAL  | 2.2  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 44  | DW    | 83   | GLU  | 2.2  |
| 29  | BH    | 95   | GLY  | 2.2  |
| 29  | DH    | 13   | GLY  | 2.2  |
| 36  | DO    | 7    | ARG  | 2.2  |
| 48  | D0    | 35   | GLY  | 2.2  |
| 19  | CS    | 5    | LEU  | 2.2  |
| 2   | CB    | 164  | ILE  | 2.2  |
| 7   | CG    | 107  | ALA  | 2.2  |
| 20  | CT    | 72   | ALA  | 2.2  |
| 41  | DT    | 83   | ALA  | 2.2  |
| 48  | D0    | 55   | ILE  | 2.2  |
| 2   | CB    | 154  | MET  | 2.2  |
| 29  | BH    | 125  | THR  | 2.2  |
| 36  | DO    | 98   | GLN  | 2.2  |
| 22  | BA    | 654  | A    | 2.2  |
| 7   | CG    | 89   | VAL  | 2.2  |
| 9   | CI    | 112  | GLU  | 2.2  |
| 41  | DT    | 67   | VAL  | 2.2  |
| 11  | CK    | 13   | ARG  | 2.2  |
| 18  | AR    | 73   | ARG  | 2.2  |
| 19  | CS    | 15   | LEU  | 2.2  |
| 22  | DA    | 275  | C    | 2.2  |
| 13  | AM    | 40   | ALA  | 2.2  |
| 27  | DF    | 104  | ILE  | 2.2  |
| 28  | DG    | 73   | ASN  | 2.2  |
| 41  | DT    | 59   | ASN  | 2.2  |
| 14  | AN    | 12   | LYS  | 2.2  |
| 18  | CR    | 48   | ARG  | 2.2  |
| 22  | BA    | 613  | A    | 2.2  |
| 22  | BA    | 2191 | A    | 2.2  |
| 27  | DF    | 97   | TRP  | 2.1  |
| 41  | DT    | 79   | ASP  | 2.1  |
| 1   | CA    | 990  | C    | 2.1  |
| 22  | DA    | 11   | C    | 2.1  |
| 22  | DA    | 1167 | C    | 2.1  |
| 33  | DL    | 103  | ILE  | 2.1  |
| 36  | DO    | 37   | ALA  | 2.1  |
| 47  | DZ    | 9    | GLN  | 2.1  |
| 1   | CA    | 1260 | G    | 2.1  |
| 16  | CP    | 76   | LYS  | 2.1  |
| 33  | DL    | 141  | LYS  | 2.1  |
| 4   | AD    | 147  | GLU  | 2.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 13  | AM    | 107  | ARG  | 2.1  |
| 41  | DT    | 90   | GLY  | 2.1  |
| 45  | DX    | 13   | VAL  | 2.1  |
| 22  | DA    | 1347 | A    | 2.1  |
| 13  | AM    | 80   | LEU  | 2.1  |
| 29  | BH    | 75   | LEU  | 2.1  |
| 38  | DQ    | 101  | PHE  | 2.1  |
| 47  | DZ    | 24   | LEU  | 2.1  |
| 3   | CC    | 80   | LYS  | 2.1  |
| 3   | CC    | 160  | ALA  | 2.1  |
| 7   | AG    | 7    | ILE  | 2.1  |
| 7   | CG    | 7    | ILE  | 2.1  |
| 18  | CR    | 21   | ILE  | 2.1  |
| 22  | DA    | 2132 | U    | 2.1  |
| 30  | BI    | 77   | ALA  | 2.1  |
| 1   | AA    | 83   | C    | 2.1  |
| 9   | AI    | 97   | GLU  | 2.1  |
| 31  | DJ    | 35   | ARG  | 2.1  |
| 13  | AM    | 30   | SER  | 2.1  |
| 22  | BA    | 1071 | G    | 2.1  |
| 23  | DB    | 54   | G    | 2.1  |
| 28  | DG    | 90   | VAL  | 2.1  |
| 33  | DL    | 65   | GLY  | 2.1  |
| 33  | DL    | 88   | GLY  | 2.1  |
| 34  | DM    | 24   | THR  | 2.1  |
| 44  | DW    | 58   | THR  | 2.1  |
| 44  | DW    | 71   | VAL  | 2.1  |
| 33  | DL    | 125  | LEU  | 2.1  |
| 40  | DS    | 36   | LEU  | 2.1  |
| 1   | CA    | 1239 | A    | 2.1  |
| 22  | DA    | 101  | A    | 2.1  |
| 2   | CB    | 134  | ALA  | 2.1  |
| 2   | CB    | 151  | ILE  | 2.1  |
| 19  | CS    | 20   | GLU  | 2.1  |
| 20  | AT    | 12   | ILE  | 2.1  |
| 20  | CT    | 81   | ALA  | 2.1  |
| 31  | DJ    | 13   | ARG  | 2.1  |
| 50  | D2    | 32   | ALA  | 2.1  |
| 1   | CA    | 1210 | C    | 2.1  |
| 20  | AT    | 20   | HIS  | 2.1  |
| 1   | CA    | 1453 | G    | 2.1  |
| 9   | CI    | 68   | LYS  | 2.1  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 12         | AL           | 15         | LYS         | 2.1         |
| 19         | AS           | 21         | LYS         | 2.1         |
| 22         | DA           | 329        | G           | 2.1         |
| 25         | DD           | 8          | LYS         | 2.1         |
| 50         | D2           | 2          | LYS         | 2.1         |
| 14         | AN           | 16         | LEU         | 2.1         |
| 19         | AS           | 5          | LEU         | 2.1         |
| 45         | DX           | 33         | LEU         | 2.1         |
| 6          | AF           | 91         | ARG         | 2.1         |
| 10         | AJ           | 35         | GLN         | 2.1         |
| 11         | AK           | 18         | ASP         | 2.1         |
| 24         | BC           | 238        | ARG         | 2.1         |
| 27         | BF           | 113        | ASP         | 2.1         |
| 53         | B5           | 60         | ARG         | 2.1         |
| 3          | AC           | 101        | ILE         | 2.1         |
| 22         | DA           | 1224       | U           | 2.1         |
| 30         | DI           | 109        | ILE         | 2.1         |
| 22         | DA           | 2800       | A           | 2.1         |
| 23         | DB           | 119        | A           | 2.1         |
| 1          | AA           | 841        | C           | 2.1         |
| 2          | CB           | 23         | TRP         | 2.1         |
| 31         | DJ           | 92         | MET         | 2.1         |
| 2          | CB           | 131        | LYS         | 2.1         |
| 3          | AC           | 39         | VAL         | 2.1         |
| 25         | DD           | 38         | LYS         | 2.1         |
| 44         | DW           | 44         | LYS         | 2.1         |
| 9          | AI           | 33         | ARG         | 2.1         |
| 12         | CL           | 38         | TYR         | 2.1         |
| 14         | AN           | 51         | LEU         | 2.1         |
| 15         | AO           | 17         | ARG         | 2.1         |
| 25         | DD           | 46         | ARG         | 2.1         |
| 1          | AA           | 84         | U           | 2.1         |
| 1          | CA           | 1240       | U           | 2.1         |
| 20         | AT           | 87         | ALA         | 2.1         |
| 23         | DB           | 53         | A           | 2.1         |
| 27         | DF           | 161        | LYS         | 2.1         |
| 1          | CA           | 1228       | C           | 2.1         |
| 16         | CP           | 2          | VAL         | 2.1         |
| 38         | DQ           | 34         | VAL         | 2.1         |
| 45         | DX           | 47         | VAL         | 2.1         |
| 21         | AU           | 47         | ARG         | 2.1         |
| 29         | BH           | 93         | SER         | 2.1         |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 2   | AB    | 114  | LEU  | 2.1  |
| 2   | AB    | 130  | THR  | 2.1  |
| 49  | D1    | 7    | GLU  | 2.1  |
| 26  | DE    | 191  | ASP  | 2.1  |
| 22  | DA    | 1082 | U    | 2.1  |
| 23  | DB    | 22   | U    | 2.1  |
| 1   | AA    | 1002 | G    | 2.1  |
| 22  | DA    | 1731 | G    | 2.1  |
| 3   | CC    | 81   | GLY  | 2.1  |
| 1   | CA    | 1145 | A    | 2.1  |
| 17  | CQ    | 11   | ARG  | 2.1  |
| 22  | BA    | 1069 | A    | 2.1  |
| 33  | DL    | 8    | PRO  | 2.1  |
| 39  | DR    | 47   | VAL  | 2.1  |
| 42  | DU    | 70   | VAL  | 2.1  |
| 1   | CA    | 87   | C    | 2.1  |
| 36  | DO    | 20   | GLU  | 2.1  |
| 36  | DO    | 97   | PHE  | 2.1  |
| 40  | DS    | 101  | SER  | 2.1  |
| 40  | DS    | 109  | ASP  | 2.1  |
| 1   | AA    | 5    | U    | 2.1  |
| 24  | DC    | 2    | ALA  | 2.1  |
| 49  | D1    | 9    | ILE  | 2.1  |
| 1   | CA    | 1276 | G    | 2.1  |
| 1   | CA    | 1300 | G    | 2.1  |
| 5   | CE    | 152  | MET  | 2.1  |
| 7   | AG    | 64   | VAL  | 2.1  |
| 13  | CM    | 97   | VAL  | 2.1  |
| 17  | CQ    | 29   | VAL  | 2.1  |
| 22  | BA    | 1179 | G    | 2.1  |
| 22  | DA    | 117  | G    | 2.1  |
| 22  | DA    | 1311 | G    | 2.1  |
| 22  | DA    | 2668 | G    | 2.1  |
| 42  | DU    | 27   | ASN  | 2.1  |
| 42  | DU    | 59   | VAL  | 2.1  |
| 1   | CA    | 461  | A    | 2.1  |
| 9   | CI    | 94   | LEU  | 2.1  |
| 30  | BI    | 72   | LYS  | 2.1  |
| 26  | DE    | 41   | GLN  | 2.1  |
| 38  | DQ    | 71   | GLN  | 2.1  |
| 1   | AA    | 1017 | U    | 2.1  |
| 1   | CA    | 89   | U    | 2.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | CA    | 1301 | U    | 2.1  |
| 2   | CB    | 125  | THR  | 2.1  |
| 19  | AS    | 77   | THR  | 2.1  |
| 26  | DE    | 175  | ILE  | 2.1  |
| 36  | DO    | 11   | ALA  | 2.1  |
| 36  | DO    | 109  | ALA  | 2.1  |
| 7   | AG    | 8    | GLY  | 2.1  |
| 10  | CJ    | 9    | ARG  | 2.1  |
| 34  | DM    | 87   | GLY  | 2.1  |
| 3   | CC    | 89   | LYS  | 2.1  |
| 7   | AG    | 141  | VAL  | 2.1  |
| 36  | DO    | 55   | GLU  | 2.1  |
| 30  | BI    | 45   | LYS  | 2.1  |
| 9   | CI    | 63   | LEU  | 2.0  |
| 19  | AS    | 10   | PHE  | 2.1  |
| 22  | DA    | 180  | G    | 2.1  |
| 22  | DA    | 2410 | G    | 2.1  |
| 1   | CA    | 90   | C    | 2.0  |
| 2   | CB    | 104  | TRP  | 2.0  |
| 8   | AH    | 54   | ASP  | 2.0  |
| 10  | AJ    | 101  | SER  | 2.0  |
| 10  | CJ    | 101  | SER  | 2.0  |
| 39  | DR    | 18   | GLN  | 2.0  |
| 13  | CM    | 68   | ASP  | 2.0  |
| 27  | DF    | 56   | ASP  | 2.0  |
| 1   | CA    | 1029 | U    | 2.0  |
| 5   | CE    | 75   | ALA  | 2.0  |
| 13  | CM    | 104  | THR  | 2.0  |
| 22  | DA    | 2833 | U    | 2.0  |
| 44  | DW    | 41   | ARG  | 2.0  |
| 10  | CJ    | 59   | LYS  | 2.0  |
| 29  | BH    | 71   | LYS  | 2.0  |
| 37  | DP    | 9    | GLU  | 2.0  |
| 25  | DD    | 1    | MET  | 2.0  |
| 19  | AS    | 16   | LEU  | 2.0  |
| 43  | DV    | 38   | LEU  | 2.0  |
| 50  | D2    | 31   | LEU  | 2.0  |
| 7   | CG    | 140  | ASP  | 2.0  |
| 19  | CS    | 36   | ARG  | 2.0  |
| 21  | AU    | 17   | ARG  | 2.0  |
| 22  | DA    | 446  | G    | 2.0  |
| 28  | DG    | 114  | ASP  | 2.0  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 37  | DP    | 42   | ALA  | 2.0  |
| 45  | DX    | 21   | ALA  | 2.0  |
| 12  | CL    | 62   | GLU  | 2.0  |
| 44  | DW    | 72   | LYS  | 2.0  |
| 9   | CI    | 111  | VAL  | 2.0  |
| 21  | AU    | 28   | VAL  | 2.0  |
| 43  | DV    | 92   | VAL  | 2.0  |
| 6   | AF    | 80   | PHE  | 2.0  |
| 34  | DM    | 17   | ASN  | 2.0  |
| 14  | CN    | 49   | GLN  | 2.0  |
| 25  | DD    | 128  | ARG  | 2.0  |
| 40  | DS    | 9    | HIS  | 2.0  |
| 49  | D1    | 6    | ARG  | 2.0  |
| 3   | CC    | 207  | ILE  | 2.0  |
| 7   | CG    | 56   | LYS  | 2.0  |
| 10  | AJ    | 14   | ASP  | 2.0  |
| 12  | CL    | 15   | LYS  | 2.0  |
| 29  | DH    | 83   | LYS  | 2.0  |
| 30  | BI    | 64   | ASP  | 2.0  |
| 36  | DO    | 2    | ASP  | 2.0  |
| 41  | DT    | 88   | LYS  | 2.0  |
| 1   | CA    | 121  | U    | 2.0  |
| 1   | CA    | 979  | C    | 2.0  |
| 1   | CA    | 1048 | G    | 2.0  |
| 1   | CA    | 1121 | U    | 2.0  |
| 1   | CA    | 1312 | G    | 2.0  |
| 14  | CN    | 101  | TRP  | 2.0  |
| 22  | BA    | 881  | G    | 2.0  |
| 22  | BA    | 1060 | U    | 2.0  |
| 22  | DA    | 70   | G    | 2.0  |
| 22  | DA    | 183  | C    | 2.0  |
| 22  | DA    | 281  | C    | 2.0  |
| 22  | DA    | 505  | A    | 2.0  |
| 37  | DP    | 31   | TRP  | 2.0  |
| 15  | AO    | 22   | THR  | 2.0  |
| 36  | DO    | 31   | THR  | 2.0  |
| 5   | CE    | 147  | MET  | 2.0  |
| 9   | CI    | 119  | ARG  | 2.0  |
| 19  | CS    | 61   | PHE  | 2.0  |
| 13  | AM    | 56   | LEU  | 2.0  |
| 2   | AB    | 167  | ASP  | 2.0  |
| 25  | DD    | 140  | HIS  | 2.0  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 27  | BF    | 116  | GLY  | 2.0  |
| 27  | DF    | 19   | GLU  | 2.0  |
| 31  | DJ    | 9    | GLU  | 2.0  |
| 13  | AM    | 36   | ALA  | 2.0  |
| 51  | D3    | 21   | GLY  | 2.0  |
| 22  | DA    | 1108 | U    | 2.0  |
| 39  | DR    | 102  | SER  | 2.0  |
| 1   | CA    | 1034 | G    | 2.0  |
| 1   | CA    | 1220 | G    | 2.0  |
| 22  | DA    | 626  | A    | 2.0  |
| 2   | AB    | 63   | ARG  | 2.0  |
| 20  | CT    | 25   | ARG  | 2.0  |
| 28  | DG    | 49   | THR  | 2.0  |
| 29  | BH    | 124  | THR  | 2.0  |
| 38  | DQ    | 39   | VAL  | 2.0  |
| 21  | CU    | 37   | PHE  | 2.0  |
| 50  | D2    | 35   | ARG  | 2.0  |
| 2   | AB    | 141  | LEU  | 2.0  |
| 4   | AD    | 148  | LYS  | 2.0  |
| 11  | AK    | 82   | LEU  | 2.0  |
| 19  | CS    | 9    | PRO  | 2.0  |
| 33  | DL    | 119  | PRO  | 2.0  |
| 41  | DT    | 68   | LYS  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

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| Mol | Type | Chain | Res  | Atoms | RSCC  | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|-------|------|-----------------------------|-------|
| 54  | MG   | DA    | 3133 | 1/1   | -0.13 | 1.03 | 105,105,105,105             | 0     |
| 54  | MG   | CA    | 1636 | 1/1   | 0.14  | 0.24 | 127,127,127,127             | 0     |
| 54  | MG   | DA    | 3077 | 1/1   | 0.14  | 0.37 | 115,115,115,115             | 0     |
| 54  | MG   | AA    | 1666 | 1/1   | 0.22  | 0.37 | 61,61,61,61                 | 0     |
| 54  | MG   | DA    | 3100 | 1/1   | 0.30  | 0.42 | 86,86,86,86                 | 0     |
| 54  | MG   | DA    | 3135 | 1/1   | 0.33  | 0.66 | 101,101,101,101             | 0     |
| 54  | MG   | DA    | 3026 | 1/1   | 0.34  | 0.49 | 100,100,100,100             | 0     |
| 54  | MG   | CA    | 1604 | 1/1   | 0.43  | 0.16 | 95,95,95,95                 | 0     |
| 54  | MG   | DA    | 3019 | 1/1   | 0.44  | 0.32 | 109,109,109,109             | 0     |
| 54  | MG   | DA    | 3062 | 1/1   | 0.46  | 0.61 | 89,89,89,89                 | 0     |
| 54  | MG   | DA    | 3029 | 1/1   | 0.46  | 0.25 | 77,77,77,77                 | 0     |
| 54  | MG   | DA    | 3003 | 1/1   | 0.48  | 0.63 | 101,101,101,101             | 0     |
| 54  | MG   | DA    | 3119 | 1/1   | 0.49  | 0.81 | 112,112,112,112             | 0     |
| 54  | MG   | CA    | 1629 | 1/1   | 0.49  | 0.10 | 89,89,89,89                 | 0     |
| 54  | MG   | DA    | 3099 | 1/1   | 0.52  | 0.39 | 91,91,91,91                 | 0     |
| 54  | MG   | AA    | 1664 | 1/1   | 0.54  | 0.71 | 49,49,49,49                 | 0     |
| 54  | MG   | CA    | 1615 | 1/1   | 0.56  | 0.18 | 52,52,52,52                 | 0     |
| 54  | MG   | CA    | 1631 | 1/1   | 0.59  | 0.23 | 101,101,101,101             | 0     |
| 54  | MG   | DA    | 3005 | 1/1   | 0.60  | 0.53 | 103,103,103,103             | 0     |
| 54  | MG   | DA    | 3046 | 1/1   | 0.60  | 0.13 | 68,68,68,68                 | 0     |
| 54  | MG   | DA    | 3028 | 1/1   | 0.60  | 1.15 | 104,104,104,104             | 0     |
| 54  | MG   | DL    | 201  | 1/1   | 0.60  | 0.52 | 68,68,68,68                 | 0     |
| 54  | MG   | DA    | 3041 | 1/1   | 0.61  | 0.45 | 72,72,72,72                 | 0     |
| 54  | MG   | DA    | 3070 | 1/1   | 0.61  | 0.18 | 108,108,108,108             | 0     |
| 54  | MG   | DA    | 3137 | 1/1   | 0.62  | 0.48 | 52,52,52,52                 | 0     |
| 54  | MG   | CA    | 1602 | 1/1   | 0.62  | 0.12 | 87,87,87,87                 | 0     |
| 54  | MG   | DA    | 3002 | 1/1   | 0.62  | 0.14 | 78,78,78,78                 | 0     |
| 54  | MG   | DA    | 3111 | 1/1   | 0.63  | 0.19 | 103,103,103,103             | 0     |
| 54  | MG   | DA    | 3078 | 1/1   | 0.65  | 0.21 | 110,110,110,110             | 0     |
| 54  | MG   | DA    | 3061 | 1/1   | 0.65  | 2.99 | 102,102,102,102             | 0     |
| 54  | MG   | AA    | 1650 | 1/1   | 0.65  | 0.34 | 61,61,61,61                 | 0     |
| 54  | MG   | CA    | 1630 | 1/1   | 0.66  | 0.34 | 120,120,120,120             | 0     |
| 54  | MG   | DA    | 3012 | 1/1   | 0.67  | 0.22 | 78,78,78,78                 | 0     |
| 54  | MG   | DB    | 203  | 1/1   | 0.67  | 0.09 | 85,85,85,85                 | 0     |
| 54  | MG   | DA    | 3071 | 1/1   | 0.67  | 0.22 | 87,87,87,87                 | 0     |
| 54  | MG   | DA    | 3103 | 1/1   | 0.67  | 0.15 | 67,67,67,67                 | 0     |
| 54  | MG   | DA    | 3147 | 1/1   | 0.68  | 0.26 | 67,67,67,67                 | 0     |
| 54  | MG   | AA    | 1658 | 1/1   | 0.68  | 0.67 | 52,52,52,52                 | 0     |
| 54  | MG   | DA    | 3093 | 1/1   | 0.68  | 0.36 | 94,94,94,94                 | 0     |
| 54  | MG   | AA    | 1618 | 1/1   | 0.68  | 0.29 | 75,75,75,75                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | DA    | 3136 | 1/1   | 0.68 | 0.18 | 94,94,94,94                 | 0     |
| 54  | MG   | DA    | 3113 | 1/1   | 0.68 | 0.58 | 72,72,72,72                 | 0     |
| 54  | MG   | DA    | 3009 | 1/1   | 0.68 | 0.20 | 91,91,91,91                 | 0     |
| 54  | MG   | BA    | 3189 | 1/1   | 0.68 | 0.21 | 48,48,48,48                 | 0     |
| 54  | MG   | AA    | 1637 | 1/1   | 0.68 | 0.14 | 81,81,81,81                 | 0     |
| 54  | MG   | AA    | 1662 | 1/1   | 0.69 | 0.46 | 58,58,58,58                 | 0     |
| 54  | MG   | CA    | 1628 | 1/1   | 0.69 | 0.31 | 99,99,99,99                 | 0     |
| 54  | MG   | DA    | 3048 | 1/1   | 0.70 | 0.32 | 123,123,123,123             | 0     |
| 54  | MG   | AA    | 1669 | 1/1   | 0.71 | 0.28 | 45,45,45,45                 | 0     |
| 54  | MG   | BA    | 3027 | 1/1   | 0.71 | 0.30 | 44,44,44,44                 | 0     |
| 54  | MG   | DA    | 3044 | 1/1   | 0.71 | 0.46 | 113,113,113,113             | 0     |
| 54  | MG   | DA    | 3092 | 1/1   | 0.71 | 0.78 | 117,117,117,117             | 0     |
| 54  | MG   | DA    | 3091 | 1/1   | 0.71 | 0.17 | 82,82,82,82                 | 0     |
| 54  | MG   | AA    | 1656 | 1/1   | 0.71 | 0.94 | 66,66,66,66                 | 0     |
| 54  | MG   | AA    | 1668 | 1/1   | 0.72 | 0.91 | 54,54,54,54                 | 0     |
| 54  | MG   | BA    | 3049 | 1/1   | 0.72 | 0.17 | 50,50,50,50                 | 0     |
| 54  | MG   | DA    | 3106 | 1/1   | 0.73 | 0.19 | 49,49,49,49                 | 0     |
| 54  | MG   | DA    | 3127 | 1/1   | 0.73 | 0.20 | 74,74,74,74                 | 0     |
| 54  | MG   | CA    | 1635 | 1/1   | 0.73 | 0.35 | 122,122,122,122             | 0     |
| 54  | MG   | DB    | 201  | 1/1   | 0.73 | 0.13 | 113,113,113,113             | 0     |
| 54  | MG   | DA    | 3162 | 1/1   | 0.73 | 0.69 | 63,63,63,63                 | 0     |
| 54  | MG   | DA    | 3010 | 1/1   | 0.74 | 0.06 | 80,80,80,80                 | 0     |
| 54  | MG   | DA    | 3145 | 1/1   | 0.74 | 0.19 | 56,56,56,56                 | 0     |
| 54  | MG   | DA    | 3104 | 1/1   | 0.74 | 0.08 | 80,80,80,80                 | 0     |
| 54  | MG   | DA    | 3095 | 1/1   | 0.74 | 0.28 | 91,91,91,91                 | 0     |
| 54  | MG   | DA    | 3034 | 1/1   | 0.75 | 0.17 | 69,69,69,69                 | 0     |
| 54  | MG   | AA    | 1661 | 1/1   | 0.75 | 0.37 | 55,55,55,55                 | 0     |
| 54  | MG   | CA    | 1632 | 1/1   | 0.75 | 0.17 | 79,79,79,79                 | 0     |
| 54  | MG   | DA    | 3084 | 1/1   | 0.76 | 0.25 | 104,104,104,104             | 0     |
| 54  | MG   | BA    | 3120 | 1/1   | 0.76 | 0.18 | 47,47,47,47                 | 0     |
| 54  | MG   | DA    | 3023 | 1/1   | 0.76 | 0.13 | 76,76,76,76                 | 0     |
| 54  | MG   | BA    | 3082 | 1/1   | 0.76 | 0.12 | 16,16,16,16                 | 0     |
| 54  | MG   | DA    | 3027 | 1/1   | 0.76 | 0.33 | 97,97,97,97                 | 0     |
| 54  | MG   | BA    | 3058 | 1/1   | 0.77 | 0.16 | 9,9,9,9                     | 0     |
| 54  | MG   | DA    | 3049 | 1/1   | 0.77 | 0.18 | 87,87,87,87                 | 0     |
| 54  | MG   | DA    | 3159 | 1/1   | 0.77 | 0.34 | 47,47,47,47                 | 0     |
| 54  | MG   | CA    | 1614 | 1/1   | 0.77 | 0.12 | 49,49,49,49                 | 0     |
| 54  | MG   | DA    | 3056 | 1/1   | 0.77 | 0.29 | 91,91,91,91                 | 0     |
| 54  | MG   | BA    | 3168 | 1/1   | 0.78 | 0.26 | 41,41,41,41                 | 0     |
| 54  | MG   | DA    | 3151 | 1/1   | 0.78 | 0.58 | 56,56,56,56                 | 0     |
| 54  | MG   | AA    | 1626 | 1/1   | 0.78 | 0.27 | 53,53,53,53                 | 0     |
| 54  | MG   | CA    | 1603 | 1/1   | 0.78 | 0.08 | 37,37,37,37                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | AA    | 1624 | 1/1   | 0.78 | 0.12 | 46,46,46,46                 | 0     |
| 54  | MG   | AA    | 1645 | 1/1   | 0.79 | 0.26 | 54,54,54,54                 | 0     |
| 54  | MG   | DA    | 3042 | 1/1   | 0.79 | 0.13 | 87,87,87,87                 | 0     |
| 54  | MG   | CA    | 1621 | 1/1   | 0.79 | 0.14 | 72,72,72,72                 | 0     |
| 54  | MG   | DA    | 3072 | 1/1   | 0.79 | 0.28 | 86,86,86,86                 | 0     |
| 54  | MG   | CA    | 1617 | 1/1   | 0.79 | 0.19 | 57,57,57,57                 | 0     |
| 54  | MG   | DA    | 3016 | 1/1   | 0.79 | 0.37 | 73,73,73,73                 | 0     |
| 54  | MG   | DA    | 3165 | 1/1   | 0.80 | 0.15 | 100,100,100,100             | 0     |
| 54  | MG   | DA    | 3088 | 1/1   | 0.80 | 0.12 | 75,75,75,75                 | 0     |
| 54  | MG   | DA    | 3045 | 1/1   | 0.80 | 0.14 | 87,87,87,87                 | 0     |
| 54  | MG   | DA    | 3144 | 1/1   | 0.80 | 0.29 | 72,72,72,72                 | 0     |
| 54  | MG   | DA    | 3014 | 1/1   | 0.80 | 0.20 | 78,78,78,78                 | 0     |
| 54  | MG   | DA    | 3132 | 1/1   | 0.80 | 0.25 | 64,64,64,64                 | 0     |
| 54  | MG   | CA    | 1606 | 1/1   | 0.80 | 0.22 | 90,90,90,90                 | 0     |
| 54  | MG   | CA    | 1649 | 1/1   | 0.80 | 0.29 | 61,61,61,61                 | 0     |
| 54  | MG   | AA    | 1638 | 1/1   | 0.81 | 0.09 | 64,64,64,64                 | 0     |
| 54  | MG   | DA    | 3140 | 1/1   | 0.81 | 0.36 | 42,42,42,42                 | 0     |
| 54  | MG   | DA    | 3125 | 1/1   | 0.81 | 0.17 | 59,59,59,59                 | 0     |
| 54  | MG   | CA    | 1608 | 1/1   | 0.81 | 0.18 | 80,80,80,80                 | 0     |
| 54  | MG   | DA    | 3143 | 1/1   | 0.81 | 0.10 | 73,73,73,73                 | 0     |
| 54  | MG   | DA    | 3057 | 1/1   | 0.81 | 0.21 | 92,92,92,92                 | 0     |
| 54  | MG   | AA    | 1659 | 1/1   | 0.81 | 0.18 | 62,62,62,62                 | 0     |
| 54  | MG   | BA    | 3134 | 1/1   | 0.81 | 0.42 | 54,54,54,54                 | 0     |
| 54  | MG   | DA    | 3098 | 1/1   | 0.81 | 0.19 | 60,60,60,60                 | 0     |
| 54  | MG   | BA    | 3085 | 1/1   | 0.81 | 0.22 | 29,29,29,29                 | 0     |
| 54  | MG   | DA    | 3126 | 1/1   | 0.82 | 0.20 | 77,77,77,77                 | 0     |
| 54  | MG   | AA    | 1639 | 1/1   | 0.82 | 0.14 | 45,45,45,45                 | 0     |
| 54  | MG   | BA    | 3194 | 1/1   | 0.82 | 0.85 | 41,41,41,41                 | 0     |
| 54  | MG   | DA    | 3038 | 1/1   | 0.82 | 0.12 | 64,64,64,64                 | 0     |
| 54  | MG   | DA    | 3060 | 1/1   | 0.82 | 0.36 | 81,81,81,81                 | 0     |
| 54  | MG   | DA    | 3134 | 1/1   | 0.82 | 0.14 | 54,54,54,54                 | 0     |
| 54  | MG   | CA    | 1637 | 1/1   | 0.82 | 0.23 | 64,64,64,64                 | 0     |
| 54  | MG   | DA    | 3080 | 1/1   | 0.82 | 0.20 | 96,96,96,96                 | 0     |
| 54  | MG   | BA    | 3005 | 1/1   | 0.82 | 0.14 | 45,45,45,45                 | 0     |
| 54  | MG   | DA    | 3017 | 1/1   | 0.82 | 0.54 | 100,100,100,100             | 0     |
| 54  | MG   | DA    | 3085 | 1/1   | 0.83 | 0.17 | 76,76,76,76                 | 0     |
| 54  | MG   | DA    | 3124 | 1/1   | 0.83 | 0.17 | 87,87,87,87                 | 0     |
| 54  | MG   | CA    | 1605 | 1/1   | 0.83 | 0.17 | 86,86,86,86                 | 0     |
| 54  | MG   | DA    | 3058 | 1/1   | 0.83 | 0.92 | 107,107,107,107             | 0     |
| 54  | MG   | DA    | 3008 | 1/1   | 0.83 | 0.30 | 102,102,102,102             | 0     |
| 54  | MG   | BA    | 3090 | 1/1   | 0.83 | 0.17 | 34,34,34,34                 | 0     |
| 54  | MG   | CA    | 1610 | 1/1   | 0.83 | 0.08 | 65,65,65,65                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | AA    | 1657 | 1/1   | 0.84 | 0.29 | 60,60,60,60                 | 0     |
| 54  | MG   | DA    | 3006 | 1/1   | 0.84 | 0.06 | 95,95,95,95                 | 0     |
| 54  | MG   | AA    | 1619 | 1/1   | 0.84 | 0.08 | 71,71,71,71                 | 0     |
| 54  | MG   | CA    | 1653 | 1/1   | 0.84 | 0.17 | 47,47,47,47                 | 0     |
| 54  | MG   | DA    | 3032 | 1/1   | 0.84 | 0.23 | 71,71,71,71                 | 0     |
| 54  | MG   | DA    | 3011 | 1/1   | 0.84 | 0.15 | 73,73,73,73                 | 0     |
| 54  | MG   | CA    | 1638 | 1/1   | 0.84 | 0.06 | 65,65,65,65                 | 0     |
| 54  | MG   | BA    | 3057 | 1/1   | 0.84 | 0.20 | 68,68,68,68                 | 0     |
| 54  | MG   | DA    | 3116 | 1/1   | 0.84 | 0.33 | 72,72,72,72                 | 0     |
| 54  | MG   | CA    | 1626 | 1/1   | 0.84 | 0.20 | 54,54,54,54                 | 0     |
| 54  | MG   | AA    | 1651 | 1/1   | 0.84 | 0.20 | 51,51,51,51                 | 0     |
| 54  | MG   | DA    | 3089 | 1/1   | 0.85 | 0.32 | 87,87,87,87                 | 0     |
| 54  | MG   | D2    | 101  | 1/1   | 0.85 | 0.17 | 76,76,76,76                 | 0     |
| 54  | MG   | CA    | 1611 | 1/1   | 0.85 | 0.25 | 87,87,87,87                 | 0     |
| 54  | MG   | DA    | 3161 | 1/1   | 0.85 | 0.30 | 46,46,46,46                 | 0     |
| 54  | MG   | DA    | 3107 | 1/1   | 0.85 | 0.12 | 70,70,70,70                 | 0     |
| 54  | MG   | BA    | 3076 | 1/1   | 0.85 | 0.17 | 33,33,33,33                 | 0     |
| 54  | MG   | DA    | 3047 | 1/1   | 0.85 | 0.11 | 74,74,74,74                 | 0     |
| 54  | MG   | DA    | 3120 | 1/1   | 0.85 | 0.18 | 81,81,81,81                 | 0     |
| 54  | MG   | DA    | 3031 | 1/1   | 0.85 | 0.14 | 65,65,65,65                 | 0     |
| 54  | MG   | DA    | 3040 | 1/1   | 0.86 | 0.12 | 80,80,80,80                 | 0     |
| 54  | MG   | BA    | 3100 | 1/1   | 0.86 | 0.29 | 51,51,51,51                 | 0     |
| 54  | MG   | DA    | 3163 | 1/1   | 0.86 | 0.26 | 64,64,64,64                 | 0     |
| 54  | MG   | CA    | 1643 | 1/1   | 0.86 | 0.30 | 44,44,44,44                 | 0     |
| 54  | MG   | BA    | 3059 | 1/1   | 0.86 | 0.35 | 36,36,36,36                 | 0     |
| 54  | MG   | AA    | 1612 | 1/1   | 0.86 | 0.11 | 48,48,48,48                 | 0     |
| 54  | MG   | AA    | 1614 | 1/1   | 0.86 | 0.23 | 74,74,74,74                 | 0     |
| 54  | MG   | BA    | 3125 | 1/1   | 0.86 | 0.29 | 39,39,39,39                 | 0     |
| 54  | MG   | DA    | 3022 | 1/1   | 0.86 | 0.07 | 55,55,55,55                 | 0     |
| 54  | MG   | DA    | 3157 | 1/1   | 0.86 | 0.67 | 76,76,76,76                 | 0     |
| 54  | MG   | AA    | 1622 | 1/1   | 0.86 | 0.18 | 50,50,50,50                 | 0     |
| 54  | MG   | DA    | 3158 | 1/1   | 0.86 | 0.23 | 52,52,52,52                 | 0     |
| 54  | MG   | DA    | 3083 | 1/1   | 0.86 | 0.23 | 74,74,74,74                 | 0     |
| 54  | MG   | DA    | 3130 | 1/1   | 0.87 | 0.24 | 80,80,80,80                 | 0     |
| 54  | MG   | DA    | 3004 | 1/1   | 0.87 | 0.08 | 78,78,78,78                 | 0     |
| 54  | MG   | BA    | 3165 | 1/1   | 0.87 | 0.22 | 38,38,38,38                 | 0     |
| 54  | MG   | DA    | 3007 | 1/1   | 0.87 | 0.34 | 119,119,119,119             | 0     |
| 54  | MG   | CA    | 1646 | 1/1   | 0.87 | 0.40 | 97,97,97,97                 | 0     |
| 54  | MG   | DA    | 3021 | 1/1   | 0.87 | 0.16 | 53,53,53,53                 | 0     |
| 54  | MG   | AA    | 1642 | 1/1   | 0.87 | 0.19 | 32,32,32,32                 | 0     |
| 54  | MG   | DA    | 3067 | 1/1   | 0.87 | 0.12 | 53,53,53,53                 | 0     |
| 54  | MG   | AA    | 1627 | 1/1   | 0.87 | 0.06 | 48,48,48,48                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | DA    | 3087 | 1/1   | 0.87 | 0.15 | 64,64,64,64                 | 0     |
| 54  | MG   | DA    | 3037 | 1/1   | 0.88 | 0.12 | 92,92,92,92                 | 0     |
| 55  | DOL  | DA    | 3001 | 48/48 | 0.88 | 0.32 | 28,49,62,81                 | 0     |
| 54  | MG   | AA    | 1665 | 1/1   | 0.88 | 0.27 | 47,47,47,47                 | 0     |
| 54  | MG   | BA    | 3146 | 1/1   | 0.88 | 0.18 | 32,32,32,32                 | 0     |
| 54  | MG   | BA    | 3078 | 1/1   | 0.88 | 0.49 | 87,87,87,87                 | 0     |
| 54  | MG   | DA    | 3055 | 1/1   | 0.88 | 0.12 | 59,59,59,59                 | 0     |
| 54  | MG   | BA    | 3104 | 1/1   | 0.88 | 0.11 | 8,8,8,8                     | 0     |
| 54  | MG   | DA    | 3150 | 1/1   | 0.88 | 0.27 | 50,50,50,50                 | 0     |
| 54  | MG   | DA    | 3081 | 1/1   | 0.88 | 0.22 | 66,66,66,66                 | 0     |
| 54  | MG   | AM    | 201  | 1/1   | 0.88 | 0.85 | 59,59,59,59                 | 0     |
| 54  | MG   | DA    | 3068 | 1/1   | 0.88 | 0.14 | 64,64,64,64                 | 0     |
| 54  | MG   | BA    | 3137 | 1/1   | 0.88 | 0.36 | 46,46,46,46                 | 0     |
| 54  | MG   | DA    | 3101 | 1/1   | 0.88 | 0.13 | 63,63,63,63                 | 0     |
| 54  | MG   | AA    | 1633 | 1/1   | 0.88 | 0.12 | 51,51,51,51                 | 0     |
| 54  | MG   | BA    | 3089 | 1/1   | 0.88 | 0.13 | 24,24,24,24                 | 0     |
| 54  | MG   | DA    | 3025 | 1/1   | 0.88 | 0.23 | 68,68,68,68                 | 0     |
| 54  | MG   | DA    | 3066 | 1/1   | 0.88 | 0.14 | 58,58,58,58                 | 0     |
| 54  | MG   | CA    | 1609 | 1/1   | 0.88 | 0.07 | 87,87,87,87                 | 0     |
| 54  | MG   | DA    | 3164 | 1/1   | 0.88 | 0.26 | 40,40,40,40                 | 0     |
| 54  | MG   | DA    | 3053 | 1/1   | 0.88 | 0.12 | 44,44,44,44                 | 0     |
| 54  | MG   | CA    | 1655 | 1/1   | 0.88 | 0.11 | 45,45,45,45                 | 0     |
| 54  | MG   | BA    | 3167 | 1/1   | 0.88 | 0.26 | 32,32,32,32                 | 0     |
| 54  | MG   | DA    | 3096 | 1/1   | 0.88 | 0.11 | 61,61,61,61                 | 0     |
| 54  | MG   | DA    | 3149 | 1/1   | 0.89 | 0.41 | 55,55,55,55                 | 0     |
| 54  | MG   | AA    | 1631 | 1/1   | 0.89 | 0.14 | 52,52,52,52                 | 0     |
| 54  | MG   | CA    | 1633 | 1/1   | 0.89 | 0.53 | 76,76,76,76                 | 0     |
| 54  | MG   | CA    | 1613 | 1/1   | 0.89 | 0.11 | 20,20,20,20                 | 0     |
| 54  | MG   | DA    | 3094 | 1/1   | 0.89 | 0.30 | 87,87,87,87                 | 0     |
| 54  | MG   | DA    | 3030 | 1/1   | 0.89 | 0.22 | 70,70,70,70                 | 0     |
| 54  | MG   | DA    | 3035 | 1/1   | 0.89 | 0.10 | 79,79,79,79                 | 0     |
| 54  | MG   | BA    | 3075 | 1/1   | 0.89 | 0.22 | 35,35,35,35                 | 0     |
| 54  | MG   | DA    | 3079 | 1/1   | 0.89 | 0.12 | 98,98,98,98                 | 0     |
| 54  | MG   | CA    | 1644 | 1/1   | 0.89 | 0.23 | 43,43,43,43                 | 0     |
| 54  | MG   | BA    | 3042 | 1/1   | 0.89 | 0.34 | 2,2,2,2                     | 0     |
| 54  | MG   | AA    | 1608 | 1/1   | 0.89 | 0.13 | 27,27,27,27                 | 0     |
| 54  | MG   | AA    | 1667 | 1/1   | 0.90 | 0.16 | 30,30,30,30                 | 0     |
| 54  | MG   | DA    | 3146 | 1/1   | 0.90 | 0.40 | 48,48,48,48                 | 0     |
| 54  | MG   | AA    | 1647 | 1/1   | 0.90 | 0.17 | 48,48,48,48                 | 0     |
| 54  | MG   | DA    | 3109 | 1/1   | 0.90 | 0.14 | 47,47,47,47                 | 0     |
| 54  | MG   | DA    | 3024 | 1/1   | 0.90 | 0.19 | 46,46,46,46                 | 0     |
| 54  | MG   | DA    | 3129 | 1/1   | 0.90 | 0.15 | 50,50,50,50                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | DA    | 3118 | 1/1   | 0.90 | 0.09 | 55,55,55,55                 | 0     |
| 54  | MG   | AA    | 1606 | 1/1   | 0.90 | 0.08 | 44,44,44,44                 | 0     |
| 54  | MG   | BA    | 3101 | 1/1   | 0.90 | 0.10 | 1,1,1,1                     | 0     |
| 54  | MG   | BA    | 3094 | 1/1   | 0.90 | 0.10 | 42,42,42,42                 | 0     |
| 54  | MG   | BA    | 3116 | 1/1   | 0.90 | 0.20 | 32,32,32,32                 | 0     |
| 54  | MG   | CA    | 1627 | 1/1   | 0.90 | 0.28 | 87,87,87,87                 | 0     |
| 54  | MG   | DA    | 3112 | 1/1   | 0.90 | 0.42 | 92,92,92,92                 | 0     |
| 54  | MG   | DA    | 3156 | 1/1   | 0.90 | 0.19 | 57,57,57,57                 | 0     |
| 54  | MG   | DA    | 3075 | 1/1   | 0.90 | 0.19 | 83,83,83,83                 | 0     |
| 54  | MG   | CA    | 1607 | 1/1   | 0.90 | 0.09 | 53,53,53,53                 | 0     |
| 54  | MG   | BA    | 3079 | 1/1   | 0.90 | 0.08 | 22,22,22,22                 | 0     |
| 54  | MG   | DA    | 3121 | 1/1   | 0.90 | 0.06 | 48,48,48,48                 | 0     |
| 54  | MG   | BA    | 3147 | 1/1   | 0.90 | 0.47 | 23,23,23,23                 | 0     |
| 54  | MG   | DA    | 3131 | 1/1   | 0.90 | 0.61 | 94,94,94,94                 | 0     |
| 54  | MG   | CA    | 1656 | 1/1   | 0.90 | 0.27 | 50,50,50,50                 | 0     |
| 54  | MG   | AA    | 1644 | 1/1   | 0.90 | 0.38 | 45,45,45,45                 | 0     |
| 54  | MG   | AA    | 1607 | 1/1   | 0.90 | 0.05 | 54,54,54,54                 | 0     |
| 54  | MG   | DA    | 3015 | 1/1   | 0.90 | 0.13 | 63,63,63,63                 | 0     |
| 54  | MG   | BA    | 3119 | 1/1   | 0.90 | 0.09 | 21,21,21,21                 | 0     |
| 54  | MG   | DA    | 3018 | 1/1   | 0.91 | 0.17 | 55,55,55,55                 | 0     |
| 54  | MG   | DA    | 3153 | 1/1   | 0.91 | 0.12 | 45,45,45,45                 | 0     |
| 54  | MG   | BA    | 3087 | 1/1   | 0.91 | 0.12 | 2,2,2,2                     | 0     |
| 54  | MG   | DA    | 3043 | 1/1   | 0.91 | 0.10 | 68,68,68,68                 | 0     |
| 54  | MG   | BA    | 3178 | 1/1   | 0.91 | 0.47 | 27,27,27,27                 | 0     |
| 54  | MG   | BA    | 3017 | 1/1   | 0.91 | 0.14 | 13,13,13,13                 | 0     |
| 54  | MG   | DA    | 3074 | 1/1   | 0.91 | 0.09 | 72,72,72,72                 | 0     |
| 54  | MG   | BA    | 3015 | 1/1   | 0.91 | 0.09 | 4,4,4,4                     | 0     |
| 54  | MG   | AA    | 1609 | 1/1   | 0.91 | 0.12 | 35,35,35,35                 | 0     |
| 54  | MG   | BA    | 3195 | 1/1   | 0.91 | 0.57 | 31,31,31,31                 | 0     |
| 54  | MG   | BA    | 3159 | 1/1   | 0.91 | 0.20 | 8,8,8,8                     | 0     |
| 54  | MG   | BA    | 3073 | 1/1   | 0.91 | 0.08 | 12,12,12,12                 | 0     |
| 54  | MG   | DA    | 3148 | 1/1   | 0.91 | 0.19 | 41,41,41,41                 | 0     |
| 54  | MG   | AA    | 1663 | 1/1   | 0.91 | 0.11 | 45,45,45,45                 | 0     |
| 54  | MG   | DA    | 3122 | 1/1   | 0.91 | 0.10 | 36,36,36,36                 | 0     |
| 54  | MG   | DA    | 3117 | 1/1   | 0.91 | 0.07 | 72,72,72,72                 | 0     |
| 54  | MG   | AA    | 1643 | 1/1   | 0.91 | 0.16 | 42,42,42,42                 | 0     |
| 54  | MG   | DA    | 3123 | 1/1   | 0.91 | 0.14 | 62,62,62,62                 | 0     |
| 54  | MG   | AA    | 1625 | 1/1   | 0.91 | 0.13 | 14,14,14,14                 | 0     |
| 54  | MG   | CA    | 1634 | 1/1   | 0.91 | 0.12 | 51,51,51,51                 | 0     |
| 54  | MG   | DA    | 3115 | 1/1   | 0.91 | 0.33 | 113,113,113,113             | 0     |
| 54  | MG   | AA    | 1630 | 1/1   | 0.92 | 0.07 | 35,35,35,35                 | 0     |
| 54  | MG   | CA    | 1642 | 1/1   | 0.92 | 0.22 | 25,25,25,25                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | BA    | 3170 | 1/1   | 0.92 | 0.15 | 36,36,36,36                 | 0     |
| 54  | MG   | BA    | 3135 | 1/1   | 0.92 | 0.12 | 3,3,3,3                     | 0     |
| 54  | MG   | BA    | 3016 | 1/1   | 0.92 | 0.34 | 51,51,51,51                 | 0     |
| 54  | MG   | DA    | 3108 | 1/1   | 0.92 | 0.19 | 61,61,61,61                 | 0     |
| 54  | MG   | BA    | 3081 | 1/1   | 0.92 | 0.11 | 18,18,18,18                 | 0     |
| 54  | MG   | BA    | 3172 | 1/1   | 0.92 | 0.09 | 27,27,27,27                 | 0     |
| 54  | MG   | AA    | 1601 | 1/1   | 0.92 | 0.10 | 53,53,53,53                 | 0     |
| 54  | MG   | BA    | 3096 | 1/1   | 0.92 | 0.09 | 19,19,19,19                 | 0     |
| 54  | MG   | BA    | 3190 | 1/1   | 0.92 | 0.14 | 39,39,39,39                 | 0     |
| 54  | MG   | AA    | 1628 | 1/1   | 0.92 | 0.24 | 59,59,59,59                 | 0     |
| 54  | MG   | AA    | 1613 | 1/1   | 0.92 | 0.12 | 33,33,33,33                 | 0     |
| 54  | MG   | BA    | 3191 | 1/1   | 0.92 | 0.29 | 12,12,12,12                 | 0     |
| 54  | MG   | DA    | 3020 | 1/1   | 0.92 | 0.22 | 49,49,49,49                 | 0     |
| 54  | MG   | BA    | 3114 | 1/1   | 0.92 | 0.12 | 0,0,0,0                     | 0     |
| 54  | MG   | CA    | 1639 | 1/1   | 0.92 | 0.08 | 49,49,49,49                 | 0     |
| 54  | MG   | BA    | 3151 | 1/1   | 0.92 | 0.20 | 12,12,12,12                 | 0     |
| 54  | MG   | DA    | 3105 | 1/1   | 0.92 | 0.21 | 81,81,81,81                 | 0     |
| 54  | MG   | DA    | 3114 | 1/1   | 0.92 | 0.14 | 66,66,66,66                 | 0     |
| 54  | MG   | DA    | 3152 | 1/1   | 0.92 | 0.10 | 45,45,45,45                 | 0     |
| 54  | MG   | DA    | 3065 | 1/1   | 0.93 | 0.10 | 34,34,34,34                 | 0     |
| 54  | MG   | CA    | 1652 | 1/1   | 0.93 | 0.15 | 86,86,86,86                 | 0     |
| 54  | MG   | DA    | 3036 | 1/1   | 0.93 | 0.17 | 62,62,62,62                 | 0     |
| 54  | MG   | BA    | 3054 | 1/1   | 0.93 | 0.09 | 6,6,6,6                     | 0     |
| 54  | MG   | BA    | 3069 | 1/1   | 0.93 | 0.16 | 1,1,1,1                     | 0     |
| 54  | MG   | BA    | 3012 | 1/1   | 0.93 | 0.08 | 19,19,19,19                 | 0     |
| 54  | MG   | CA    | 1624 | 1/1   | 0.93 | 0.07 | 39,39,39,39                 | 0     |
| 54  | MG   | DB    | 202  | 1/1   | 0.93 | 0.10 | 64,64,64,64                 | 0     |
| 54  | MG   | AA    | 1660 | 1/1   | 0.93 | 0.34 | 45,45,45,45                 | 0     |
| 54  | MG   | CA    | 1601 | 1/1   | 0.93 | 0.11 | 38,38,38,38                 | 0     |
| 54  | MG   | AA    | 1604 | 1/1   | 0.93 | 0.11 | 56,56,56,56                 | 0     |
| 54  | MG   | BA    | 3140 | 1/1   | 0.93 | 0.33 | 0,0,0,0                     | 0     |
| 54  | MG   | BA    | 3156 | 1/1   | 0.93 | 0.35 | 26,26,26,26                 | 0     |
| 54  | MG   | BA    | 3105 | 1/1   | 0.93 | 0.10 | 10,10,10,10                 | 0     |
| 54  | MG   | BA    | 3103 | 1/1   | 0.93 | 0.16 | 0,0,0,0                     | 0     |
| 54  | MG   | BA    | 3164 | 1/1   | 0.93 | 0.12 | 4,4,4,4                     | 0     |
| 54  | MG   | BA    | 3169 | 1/1   | 0.93 | 0.16 | 29,29,29,29                 | 0     |
| 54  | MG   | AA    | 1632 | 1/1   | 0.93 | 0.06 | 37,37,37,37                 | 0     |
| 54  | MG   | BA    | 3122 | 1/1   | 0.93 | 0.11 | 25,25,25,25                 | 0     |
| 54  | MG   | BA    | 3040 | 1/1   | 0.93 | 0.14 | 2,2,2,2                     | 0     |
| 54  | MG   | BA    | 3031 | 1/1   | 0.93 | 0.10 | 20,20,20,20                 | 0     |
| 54  | MG   | BA    | 3121 | 1/1   | 0.93 | 0.09 | 2,2,2,2                     | 0     |
| 54  | MG   | BA    | 3095 | 1/1   | 0.93 | 0.07 | 17,17,17,17                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | BA    | 3136 | 1/1   | 0.93 | 0.17 | 24,24,24,24                 | 0     |
| 54  | MG   | AA    | 1603 | 1/1   | 0.93 | 0.14 | 44,44,44,44                 | 0     |
| 54  | MG   | BA    | 3180 | 1/1   | 0.93 | 0.14 | 29,29,29,29                 | 0     |
| 54  | MG   | BA    | 3047 | 1/1   | 0.93 | 0.17 | 4,4,4,4                     | 0     |
| 54  | MG   | AA    | 1610 | 1/1   | 0.93 | 0.29 | 65,65,65,65                 | 0     |
| 54  | MG   | BA    | 3036 | 1/1   | 0.93 | 0.14 | 10,10,10,10                 | 0     |
| 54  | MG   | DA    | 3139 | 1/1   | 0.93 | 0.26 | 31,31,31,31                 | 0     |
| 54  | MG   | DA    | 3069 | 1/1   | 0.93 | 0.17 | 80,80,80,80                 | 0     |
| 54  | MG   | BA    | 3149 | 1/1   | 0.93 | 0.23 | 44,44,44,44                 | 0     |
| 54  | MG   | DA    | 3110 | 1/1   | 0.93 | 0.23 | 39,39,39,39                 | 0     |
| 54  | MG   | BA    | 3052 | 1/1   | 0.93 | 0.08 | 7,7,7,7                     | 0     |
| 54  | MG   | DA    | 3073 | 1/1   | 0.93 | 0.31 | 61,61,61,61                 | 0     |
| 54  | MG   | DA    | 3142 | 1/1   | 0.93 | 0.13 | 34,34,34,34                 | 0     |
| 54  | MG   | BA    | 3150 | 1/1   | 0.94 | 0.14 | 29,29,29,29                 | 0     |
| 54  | MG   | BA    | 3050 | 1/1   | 0.94 | 0.07 | 18,18,18,18                 | 0     |
| 54  | MG   | AA    | 1602 | 1/1   | 0.94 | 0.42 | 55,55,55,55                 | 0     |
| 54  | MG   | AA    | 1634 | 1/1   | 0.94 | 0.43 | 73,73,73,73                 | 0     |
| 54  | MG   | CA    | 1622 | 1/1   | 0.94 | 0.16 | 46,46,46,46                 | 0     |
| 54  | MG   | AA    | 1654 | 1/1   | 0.94 | 0.14 | 34,34,34,34                 | 0     |
| 54  | MG   | BA    | 3014 | 1/1   | 0.94 | 0.14 | 0,0,0,0                     | 0     |
| 54  | MG   | CA    | 1651 | 1/1   | 0.94 | 0.16 | 42,42,42,42                 | 0     |
| 54  | MG   | AA    | 1616 | 1/1   | 0.94 | 0.08 | 57,57,57,57                 | 0     |
| 54  | MG   | BA    | 3141 | 1/1   | 0.94 | 0.14 | 17,17,17,17                 | 0     |
| 54  | MG   | DA    | 3033 | 1/1   | 0.94 | 0.16 | 63,63,63,63                 | 0     |
| 54  | MG   | BA    | 3161 | 1/1   | 0.94 | 0.16 | 33,33,33,33                 | 0     |
| 54  | MG   | CA    | 1648 | 1/1   | 0.94 | 0.25 | 19,19,19,19                 | 0     |
| 54  | MG   | BA    | 3062 | 1/1   | 0.94 | 0.32 | 46,46,46,46                 | 0     |
| 54  | MG   | DA    | 3064 | 1/1   | 0.94 | 0.17 | 53,53,53,53                 | 0     |
| 54  | MG   | BA    | 3063 | 1/1   | 0.94 | 0.53 | 52,52,52,52                 | 0     |
| 54  | MG   | DA    | 3128 | 1/1   | 0.94 | 0.12 | 79,79,79,79                 | 0     |
| 54  | MG   | DA    | 3090 | 1/1   | 0.94 | 0.07 | 84,84,84,84                 | 0     |
| 54  | MG   | BA    | 3162 | 1/1   | 0.94 | 0.11 | 21,21,21,21                 | 0     |
| 54  | MG   | DA    | 3082 | 1/1   | 0.94 | 0.10 | 59,59,59,59                 | 0     |
| 54  | MG   | DA    | 3063 | 1/1   | 0.94 | 0.17 | 50,50,50,50                 | 0     |
| 54  | MG   | DA    | 3054 | 1/1   | 0.94 | 0.11 | 48,48,48,48                 | 0     |
| 54  | MG   | DA    | 3013 | 1/1   | 0.94 | 0.18 | 45,45,45,45                 | 0     |
| 54  | MG   | DA    | 3059 | 1/1   | 0.94 | 0.11 | 39,39,39,39                 | 0     |
| 54  | MG   | BA    | 3086 | 1/1   | 0.94 | 0.15 | 24,24,24,24                 | 0     |
| 54  | MG   | BA    | 3002 | 1/1   | 0.94 | 0.06 | 19,19,19,19                 | 0     |
| 54  | MG   | AA    | 1653 | 1/1   | 0.94 | 0.25 | 47,47,47,47                 | 0     |
| 54  | MG   | BA    | 3032 | 1/1   | 0.94 | 0.18 | 5,5,5,5                     | 0     |
| 54  | MG   | BA    | 3152 | 1/1   | 0.94 | 0.18 | 12,12,12,12                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | DA    | 3138 | 1/1   | 0.94 | 0.22 | 38,38,38,38                 | 0     |
| 54  | MG   | BA    | 3113 | 1/1   | 0.94 | 0.15 | 39,39,39,39                 | 0     |
| 54  | MG   | CA    | 1641 | 1/1   | 0.94 | 0.26 | 66,66,66,66                 | 0     |
| 54  | MG   | DA    | 3160 | 1/1   | 0.94 | 0.26 | 64,64,64,64                 | 0     |
| 54  | MG   | AA    | 1629 | 1/1   | 0.94 | 0.28 | 79,79,79,79                 | 0     |
| 54  | MG   | AN    | 201  | 1/1   | 0.94 | 0.19 | 62,62,62,62                 | 0     |
| 54  | MG   | BA    | 3035 | 1/1   | 0.95 | 0.15 | 3,3,3,3                     | 0     |
| 54  | MG   | BA    | 3056 | 1/1   | 0.95 | 0.10 | 2,2,2,2                     | 0     |
| 54  | MG   | CA    | 1616 | 1/1   | 0.95 | 0.09 | 38,38,38,38                 | 0     |
| 54  | MG   | AA    | 1617 | 1/1   | 0.95 | 0.06 | 42,42,42,42                 | 0     |
| 54  | MG   | BA    | 3181 | 1/1   | 0.95 | 0.14 | 16,16,16,16                 | 0     |
| 54  | MG   | BA    | 3044 | 1/1   | 0.95 | 0.11 | 3,3,3,3                     | 0     |
| 54  | MG   | CA    | 1623 | 1/1   | 0.95 | 0.19 | 50,50,50,50                 | 0     |
| 54  | MG   | AA    | 1623 | 1/1   | 0.95 | 0.10 | 41,41,41,41                 | 0     |
| 54  | MG   | BB    | 202  | 1/1   | 0.95 | 0.08 | 6,6,6,6                     | 0     |
| 54  | MG   | BA    | 3143 | 1/1   | 0.95 | 0.31 | 22,22,22,22                 | 0     |
| 54  | MG   | BA    | 3038 | 1/1   | 0.95 | 0.16 | 31,31,31,31                 | 0     |
| 54  | MG   | BA    | 3033 | 1/1   | 0.95 | 0.10 | 9,9,9,9                     | 0     |
| 54  | MG   | BA    | 3071 | 1/1   | 0.95 | 0.19 | 66,66,66,66                 | 0     |
| 54  | MG   | BA    | 3093 | 1/1   | 0.95 | 0.15 | 57,57,57,57                 | 0     |
| 54  | MG   | BA    | 3171 | 1/1   | 0.95 | 0.15 | 28,28,28,28                 | 0     |
| 54  | MG   | DA    | 3052 | 1/1   | 0.95 | 0.10 | 60,60,60,60                 | 0     |
| 54  | MG   | BA    | 3061 | 1/1   | 0.95 | 0.27 | 40,40,40,40                 | 0     |
| 54  | MG   | DA    | 3102 | 1/1   | 0.95 | 0.14 | 61,61,61,61                 | 0     |
| 54  | MG   | BA    | 3060 | 1/1   | 0.95 | 0.07 | 14,14,14,14                 | 0     |
| 54  | MG   | BB    | 203  | 1/1   | 0.95 | 0.04 | 8,8,8,8                     | 0     |
| 54  | MG   | BA    | 3112 | 1/1   | 0.95 | 0.06 | 29,29,29,29                 | 0     |
| 54  | MG   | CA    | 1612 | 1/1   | 0.95 | 0.20 | 46,46,46,46                 | 0     |
| 54  | MG   | BB    | 201  | 1/1   | 0.95 | 0.07 | 31,31,31,31                 | 0     |
| 54  | MG   | DQ    | 201  | 1/1   | 0.95 | 0.27 | 37,37,37,37                 | 0     |
| 54  | MG   | AA    | 1670 | 1/1   | 0.95 | 0.39 | 58,58,58,58                 | 0     |
| 54  | MG   | BA    | 3174 | 1/1   | 0.95 | 0.12 | 14,14,14,14                 | 0     |
| 54  | MG   | BA    | 3080 | 1/1   | 0.95 | 0.07 | 42,42,42,42                 | 0     |
| 54  | MG   | BA    | 3020 | 1/1   | 0.95 | 0.07 | 24,24,24,24                 | 0     |
| 54  | MG   | BA    | 3183 | 1/1   | 0.95 | 0.16 | 19,19,19,19                 | 0     |
| 54  | MG   | BB    | 204  | 1/1   | 0.95 | 0.41 | 12,12,12,12                 | 0     |
| 54  | MG   | CA    | 1640 | 1/1   | 0.95 | 0.13 | 27,27,27,27                 | 0     |
| 54  | MG   | BA    | 3009 | 1/1   | 0.95 | 0.13 | 4,4,4,4                     | 0     |
| 54  | MG   | BA    | 3115 | 1/1   | 0.95 | 0.14 | 17,17,17,17                 | 0     |
| 54  | MG   | DA    | 3097 | 1/1   | 0.95 | 0.21 | 87,87,87,87                 | 0     |
| 54  | MG   | BA    | 3007 | 1/1   | 0.95 | 0.10 | 24,24,24,24                 | 0     |
| 54  | MG   | BA    | 3179 | 1/1   | 0.95 | 0.33 | 30,30,30,30                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | BA    | 3066 | 1/1   | 0.96 | 0.14 | 0,0,0,0                     | 0     |
| 54  | MG   | BA    | 3163 | 1/1   | 0.96 | 0.39 | 12,12,12,12                 | 0     |
| 54  | MG   | BA    | 3092 | 1/1   | 0.96 | 0.09 | 21,21,21,21                 | 0     |
| 54  | MG   | BA    | 3043 | 1/1   | 0.96 | 0.12 | 5,5,5,5                     | 0     |
| 54  | MG   | BA    | 3133 | 1/1   | 0.96 | 0.20 | 39,39,39,39                 | 0     |
| 54  | MG   | AA    | 1640 | 1/1   | 0.96 | 0.10 | 21,21,21,21                 | 0     |
| 54  | MG   | BA    | 3176 | 1/1   | 0.96 | 0.08 | 28,28,28,28                 | 0     |
| 54  | MG   | AA    | 1635 | 1/1   | 0.96 | 0.05 | 23,23,23,23                 | 0     |
| 54  | MG   | BA    | 3129 | 1/1   | 0.96 | 0.15 | 3,3,3,3                     | 0     |
| 54  | MG   | BA    | 3127 | 1/1   | 0.96 | 0.12 | 5,5,5,5                     | 0     |
| 54  | MG   | BA    | 3166 | 1/1   | 0.96 | 0.13 | 23,23,23,23                 | 0     |
| 54  | MG   | CA    | 1625 | 1/1   | 0.96 | 0.13 | 17,17,17,17                 | 0     |
| 54  | MG   | BA    | 3004 | 1/1   | 0.96 | 0.07 | 22,22,22,22                 | 0     |
| 54  | MG   | BA    | 3030 | 1/1   | 0.96 | 0.14 | 6,6,6,6                     | 0     |
| 54  | MG   | BA    | 3173 | 1/1   | 0.96 | 0.15 | 38,38,38,38                 | 0     |
| 54  | MG   | BA    | 3098 | 1/1   | 0.96 | 0.08 | 3,3,3,3                     | 0     |
| 54  | MG   | BA    | 3097 | 1/1   | 0.96 | 0.06 | 8,8,8,8                     | 0     |
| 54  | MG   | DA    | 3039 | 1/1   | 0.96 | 0.07 | 57,57,57,57                 | 0     |
| 54  | MG   | CA    | 1647 | 1/1   | 0.96 | 0.09 | 36,36,36,36                 | 0     |
| 54  | MG   | CA    | 1645 | 1/1   | 0.96 | 0.14 | 28,28,28,28                 | 0     |
| 54  | MG   | BA    | 3145 | 1/1   | 0.96 | 0.27 | 17,17,17,17                 | 0     |
| 54  | MG   | CA    | 1619 | 1/1   | 0.96 | 0.09 | 34,34,34,34                 | 0     |
| 54  | MG   | BA    | 3138 | 1/1   | 0.96 | 0.37 | 1,1,1,1                     | 0     |
| 54  | MG   | BA    | 3021 | 1/1   | 0.96 | 0.27 | 0,0,0,0                     | 0     |
| 54  | MG   | AA    | 1605 | 1/1   | 0.96 | 0.17 | 26,26,26,26                 | 0     |
| 54  | MG   | BA    | 3091 | 1/1   | 0.96 | 0.09 | 4,4,4,4                     | 0     |
| 54  | MG   | DA    | 3155 | 1/1   | 0.96 | 0.32 | 42,42,42,42                 | 0     |
| 54  | MG   | DA    | 3141 | 1/1   | 0.96 | 0.21 | 39,39,39,39                 | 0     |
| 54  | MG   | BA    | 3064 | 1/1   | 0.96 | 0.14 | 1,1,1,1                     | 0     |
| 54  | MG   | CA    | 1654 | 1/1   | 0.96 | 0.19 | 55,55,55,55                 | 0     |
| 55  | DOL  | BA    | 3001 | 48/48 | 0.96 | 0.20 | 1,7,30,58                   | 0     |
| 54  | MG   | BA    | 3175 | 1/1   | 0.96 | 0.13 | 34,34,34,34                 | 0     |
| 54  | MG   | BA    | 3022 | 1/1   | 0.96 | 0.07 | 16,16,16,16                 | 0     |
| 54  | MG   | BA    | 3008 | 1/1   | 0.96 | 0.15 | 33,33,33,33                 | 0     |
| 54  | MG   | BA    | 3013 | 1/1   | 0.96 | 0.22 | 0,0,0,0                     | 0     |
| 54  | MG   | BA    | 3157 | 1/1   | 0.96 | 0.07 | 18,18,18,18                 | 0     |
| 54  | MG   | BA    | 3124 | 1/1   | 0.96 | 0.10 | 20,20,20,20                 | 0     |
| 54  | MG   | BA    | 3192 | 1/1   | 0.96 | 0.18 | 23,23,23,23                 | 0     |
| 54  | MG   | AA    | 1611 | 1/1   | 0.96 | 0.07 | 20,20,20,20                 | 0     |
| 54  | MG   | DA    | 3154 | 1/1   | 0.97 | 0.45 | 57,57,57,57                 | 0     |
| 54  | MG   | BA    | 3034 | 1/1   | 0.97 | 0.13 | 2,2,2,2                     | 0     |
| 54  | MG   | BA    | 3187 | 1/1   | 0.97 | 0.15 | 30,30,30,30                 | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | BA    | 3106 | 1/1   | 0.97 | 0.18 | 5,5,5,5                     | 0     |
| 54  | MG   | DA    | 3076 | 1/1   | 0.97 | 0.07 | 66,66,66,66                 | 0     |
| 54  | MG   | BA    | 3107 | 1/1   | 0.97 | 0.19 | 0,0,0,0                     | 0     |
| 54  | MG   | BA    | 3153 | 1/1   | 0.97 | 0.10 | 26,26,26,26                 | 0     |
| 54  | MG   | BA    | 3186 | 1/1   | 0.97 | 0.20 | 14,14,14,14                 | 0     |
| 54  | MG   | BA    | 3102 | 1/1   | 0.97 | 0.08 | 9,9,9,9                     | 0     |
| 54  | MG   | BA    | 3155 | 1/1   | 0.97 | 0.10 | 18,18,18,18                 | 0     |
| 54  | MG   | BA    | 3132 | 1/1   | 0.97 | 0.16 | 27,27,27,27                 | 0     |
| 54  | MG   | BA    | 3110 | 1/1   | 0.97 | 0.20 | 4,4,4,4                     | 0     |
| 54  | MG   | BA    | 3077 | 1/1   | 0.97 | 0.13 | 12,12,12,12                 | 0     |
| 54  | MG   | AA    | 1652 | 1/1   | 0.97 | 0.18 | 18,18,18,18                 | 0     |
| 54  | MG   | BA    | 3026 | 1/1   | 0.97 | 0.11 | 3,3,3,3                     | 0     |
| 54  | MG   | BA    | 3011 | 1/1   | 0.97 | 0.08 | 0,0,0,0                     | 0     |
| 54  | MG   | BA    | 3158 | 1/1   | 0.97 | 0.25 | 22,22,22,22                 | 0     |
| 54  | MG   | AA    | 1649 | 1/1   | 0.97 | 0.14 | 32,32,32,32                 | 0     |
| 54  | MG   | BA    | 3188 | 1/1   | 0.97 | 0.14 | 6,6,6,6                     | 0     |
| 54  | MG   | BA    | 3070 | 1/1   | 0.97 | 0.14 | 0,0,0,0                     | 0     |
| 54  | MG   | AA    | 1615 | 1/1   | 0.97 | 0.11 | 62,62,62,62                 | 0     |
| 54  | MG   | BA    | 3055 | 1/1   | 0.97 | 0.18 | 0,0,0,0                     | 0     |
| 54  | MG   | BA    | 3045 | 1/1   | 0.97 | 0.06 | 27,27,27,27                 | 0     |
| 54  | MG   | BA    | 3154 | 1/1   | 0.97 | 0.14 | 12,12,12,12                 | 0     |
| 54  | MG   | CA    | 1620 | 1/1   | 0.97 | 0.04 | 61,61,61,61                 | 0     |
| 54  | MG   | BA    | 3193 | 1/1   | 0.97 | 0.21 | 32,32,32,32                 | 0     |
| 54  | MG   | BA    | 3074 | 1/1   | 0.97 | 0.12 | 1,1,1,1                     | 0     |
| 54  | MG   | CA    | 1650 | 1/1   | 0.97 | 0.09 | 42,42,42,42                 | 0     |
| 54  | MG   | BA    | 3003 | 1/1   | 0.97 | 0.08 | 18,18,18,18                 | 0     |
| 54  | MG   | BA    | 3182 | 1/1   | 0.97 | 0.16 | 16,16,16,16                 | 0     |
| 54  | MG   | BA    | 3018 | 1/1   | 0.97 | 0.19 | 0,0,0,0                     | 0     |
| 54  | MG   | BA    | 3160 | 1/1   | 0.97 | 0.10 | 3,3,3,3                     | 0     |
| 54  | MG   | BA    | 3148 | 1/1   | 0.97 | 0.17 | 28,28,28,28                 | 0     |
| 54  | MG   | BA    | 3023 | 1/1   | 0.97 | 0.08 | 1,1,1,1                     | 0     |
| 54  | MG   | AA    | 1648 | 1/1   | 0.97 | 0.16 | 33,33,33,33                 | 0     |
| 54  | MG   | AA    | 1620 | 1/1   | 0.97 | 0.06 | 30,30,30,30                 | 0     |
| 54  | MG   | BA    | 3046 | 1/1   | 0.97 | 0.15 | 6,6,6,6                     | 0     |
| 54  | MG   | BA    | 3131 | 1/1   | 0.98 | 0.24 | 1,1,1,1                     | 0     |
| 54  | MG   | CA    | 1618 | 1/1   | 0.98 | 0.16 | 35,35,35,35                 | 0     |
| 54  | MG   | DA    | 3086 | 1/1   | 0.98 | 0.10 | 74,74,74,74                 | 0     |
| 54  | MG   | BA    | 3084 | 1/1   | 0.98 | 0.08 | 16,16,16,16                 | 0     |
| 54  | MG   | BA    | 3053 | 1/1   | 0.98 | 0.10 | 6,6,6,6                     | 0     |
| 54  | MG   | BA    | 3130 | 1/1   | 0.98 | 0.14 | 0,0,0,0                     | 0     |
| 54  | MG   | BA    | 3118 | 1/1   | 0.98 | 0.12 | 4,4,4,4                     | 0     |
| 54  | MG   | DA    | 3050 | 1/1   | 0.98 | 0.10 | 48,48,48,48                 | 0     |

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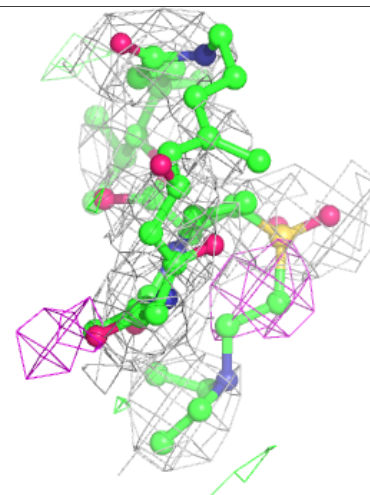
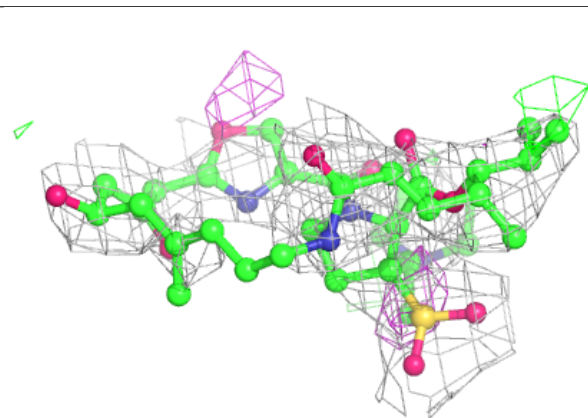
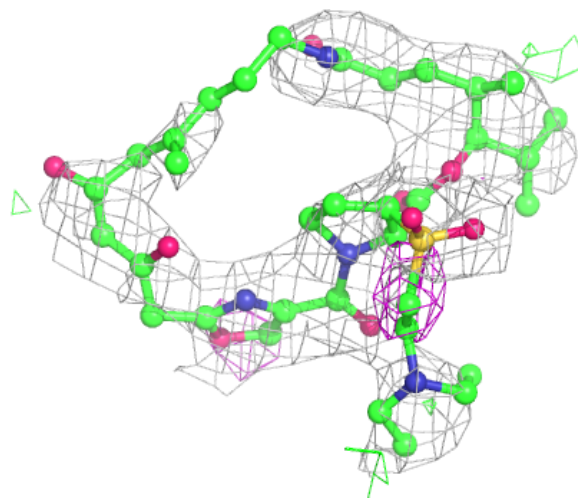
| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 54  | MG   | BA    | 3048 | 1/1   | 0.98 | 0.16 | 9,9,9,9                     | 0     |
| 56  | ZN   | D4    | 101  | 1/1   | 0.98 | 0.06 | 91,91,91,91                 | 0     |
| 54  | MG   | BA    | 3142 | 1/1   | 0.98 | 0.37 | 0,0,0,0                     | 0     |
| 54  | MG   | BA    | 3072 | 1/1   | 0.98 | 0.08 | 7,7,7,7                     | 0     |
| 54  | MG   | BA    | 3128 | 1/1   | 0.98 | 0.07 | 0,0,0,0                     | 0     |
| 54  | MG   | BA    | 3177 | 1/1   | 0.98 | 0.19 | 12,12,12,12                 | 0     |
| 54  | MG   | AA    | 1646 | 1/1   | 0.98 | 0.07 | 54,54,54,54                 | 0     |
| 54  | MG   | AA    | 1636 | 1/1   | 0.98 | 0.09 | 17,17,17,17                 | 0     |
| 54  | MG   | BA    | 3139 | 1/1   | 0.98 | 0.36 | 0,0,0,0                     | 0     |
| 54  | MG   | BA    | 3051 | 1/1   | 0.98 | 0.12 | 1,1,1,1                     | 0     |
| 54  | MG   | BA    | 3123 | 1/1   | 0.98 | 0.18 | 0,0,0,0                     | 0     |
| 54  | MG   | AA    | 1655 | 1/1   | 0.98 | 0.11 | 44,44,44,44                 | 0     |
| 54  | MG   | BA    | 3099 | 1/1   | 0.98 | 0.04 | 5,5,5,5                     | 0     |
| 54  | MG   | BA    | 3126 | 1/1   | 0.98 | 0.17 | 4,4,4,4                     | 0     |
| 54  | MG   | AA    | 1621 | 1/1   | 0.98 | 0.17 | 19,19,19,19                 | 0     |
| 54  | MG   | BA    | 3025 | 1/1   | 0.98 | 0.17 | 2,2,2,2                     | 0     |
| 54  | MG   | BQ    | 201  | 1/1   | 0.98 | 0.14 | 7,7,7,7                     | 0     |
| 54  | MG   | BA    | 3029 | 1/1   | 0.98 | 0.13 | 23,23,23,23                 | 0     |
| 54  | MG   | BA    | 3185 | 1/1   | 0.98 | 0.11 | 13,13,13,13                 | 0     |
| 54  | MG   | DA    | 3051 | 1/1   | 0.98 | 0.10 | 32,32,32,32                 | 0     |
| 54  | MG   | BA    | 3109 | 1/1   | 0.99 | 0.16 | 6,6,6,6                     | 0     |
| 54  | MG   | BA    | 3065 | 1/1   | 0.99 | 0.17 | 1,1,1,1                     | 0     |
| 54  | MG   | BA    | 3028 | 1/1   | 0.99 | 0.04 | 6,6,6,6                     | 0     |
| 54  | MG   | BA    | 3024 | 1/1   | 0.99 | 0.12 | 0,0,0,0                     | 0     |
| 54  | MG   | BA    | 3010 | 1/1   | 0.99 | 0.09 | 0,0,0,0                     | 0     |
| 54  | MG   | BA    | 3041 | 1/1   | 0.99 | 0.14 | 2,2,2,2                     | 0     |
| 54  | MG   | BA    | 3068 | 1/1   | 0.99 | 0.14 | 1,1,1,1                     | 0     |
| 54  | MG   | BA    | 3144 | 1/1   | 0.99 | 0.28 | 6,6,6,6                     | 0     |
| 54  | MG   | AA    | 1641 | 1/1   | 0.99 | 0.07 | 24,24,24,24                 | 0     |
| 54  | MG   | BA    | 3019 | 1/1   | 0.99 | 0.07 | 14,14,14,14                 | 0     |
| 54  | MG   | BA    | 3083 | 1/1   | 0.99 | 0.14 | 2,2,2,2                     | 0     |
| 54  | MG   | BA    | 3067 | 1/1   | 0.99 | 0.11 | 1,1,1,1                     | 0     |
| 54  | MG   | BA    | 3006 | 1/1   | 0.99 | 0.10 | 43,43,43,43                 | 0     |
| 54  | MG   | BA    | 3111 | 1/1   | 0.99 | 0.15 | 4,4,4,4                     | 0     |
| 54  | MG   | BA    | 3184 | 1/1   | 0.99 | 0.16 | 3,3,3,3                     | 0     |
| 54  | MG   | BA    | 3088 | 1/1   | 0.99 | 0.21 | 2,2,2,2                     | 0     |
| 54  | MG   | BA    | 3117 | 1/1   | 0.99 | 0.16 | 2,2,2,2                     | 0     |
| 54  | MG   | BA    | 3037 | 1/1   | 1.00 | 0.16 | 0,0,0,0                     | 0     |
| 56  | ZN   | B4    | 101  | 1/1   | 1.00 | 0.06 | 36,36,36,36                 | 0     |
| 54  | MG   | BA    | 3039 | 1/1   | 1.00 | 0.23 | 0,0,0,0                     | 0     |
| 54  | MG   | BA    | 3108 | 1/1   | 1.00 | 0.20 | 1,1,1,1                     | 0     |

The following is a graphical depiction of the model fit to experimental electron density of all

instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

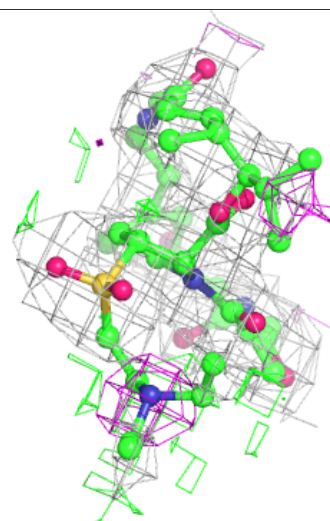
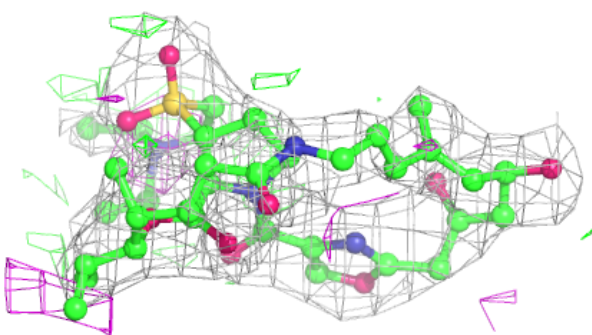
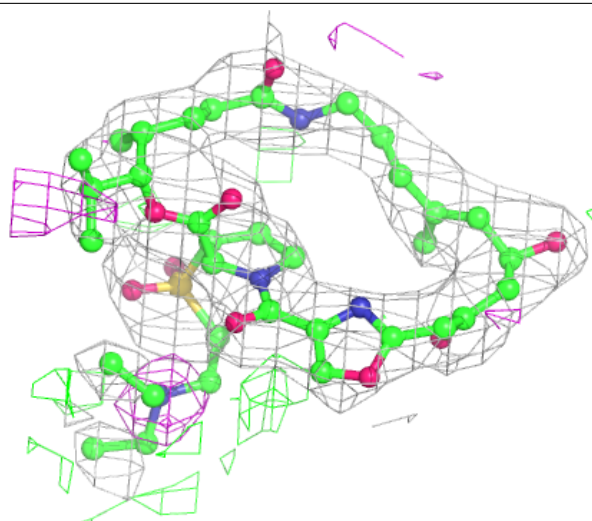
**Electron density around DOL DA 3001:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around DOL BA 3001:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.